



# **STIC Search Report**

## **Biotech-Chem Library**

**STIC Database Tracking Number: 115489**

**TO: Dwayne C Jones**  
**Location: REM/4C70**  
**Art Unit: 1614**  
**Friday, February 27, 2004**

**Case Serial Number: 10/613798**

**From: Barb O'Bryen**  
**Location: Biotech-Chem Library**  
**Remsen E01A69**  
**Phone: 571-272-2518** *AOB*

**barbara.obryen@uspto.gov**

### **Search Notes**

# SEARCH REQUEST FORM

115489

Requestor's  
Name:

Wayne C. Jones

Serial

Number:

3210/43, 748

Date:

27 FEB 84

Phone:

2-0578

Art Unit:

1614

## Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).

Please read claim 1, 4, 5 and 6

## STAFF USE ONLY

Date completed:

2 27-04

Searcher:

1118

Terminal time:

29

Elapsed time:

25

CPU time:

Total time:

Number of Searches:

Number of Databases:

Search Site

STIC

CM-1

Pre-S

Type of Search

N.A. Sequence

A.A. Sequence

Structure

Bibliographic

Vendors

IG Suite

479 STN

Dialog

APS

Geninfo

SDC

DARC/Questel

Other

=> fil reg; d stat que 17; fil capl; d que nos 18; fil uspatf; d que nos 19  
FILE 'REGISTRY' ENTERED AT 16:13:14 ON 27 FEB 2004  
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Property values tagged with IC are from the ZIC/VINITI data file  
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STRUCTURE FILE UPDATES: 25 FEB 2004 HIGHEST RN 654632-96-9  
DICTIONARY FILE UPDATES: 25 FEB 2004 HIGHEST RN 654632-96-9

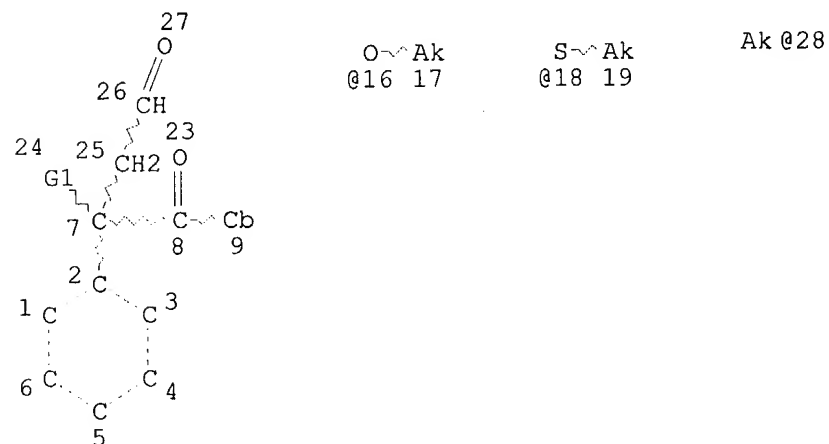
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

L3 STR



VAR G1=H/28/16/18

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 17

CONNECT IS E1 RC AT 19

CONNECT IS E1 RC AT 28

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

L7 16 SEA FILE=REGISTRY SSS FUL L3

100.0% PROCESSED 18781 ITERATIONS  
SEARCH TIME: 00.00.01

16 ANSWERS

FILE 'CAPLUS' ENTERED AT 16:13:14 ON 27 FEB 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 27 Feb 2004 VOL 140 ISS 10  
FILE LAST UPDATED: 26 Feb 2004 (20040226/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

L3 STR  
L7 16 SEA FILE=REGISTRY SSS FUL L3  
L8 15 SEA FILE=CAPLUS ABB=ON L7

FILE 'USPATFULL' ENTERED AT 16:13:14 ON 27 FEB 2004  
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 26 Feb 2004 (20040226/PD)  
FILE LAST UPDATED: 26 Feb 2004 (20040226/ED)  
HIGHEST GRANTED PATENT NUMBER: US6698023  
HIGHEST APPLICATION PUBLICATION NUMBER: US2004040063  
CA INDEXING IS CURRENT THROUGH 26 Feb 2004 (20040226/UPCA)  
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 26 Feb 2004 (20040226/PD)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2003  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2003

>>> USPAT2 is now available. USPATFULL contains full text of the <<<  
>>> original, i.e., the earliest published granted patents or <<<  
>>> applications. USPAT2 contains full text of the latest US <<<  
>>> publications, starting in 2001, for the inventions covered in <<<  
>>> USPATFULL. A USPATFULL record contains not only the original <<<  
>>> published document but also a list of any subsequent <<<  
>>> publications. The publication number, patent kind code, and <<<  
>>> publication date for all the US publications for an invention <<<  
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<  
>>> records and may be searched in standard search fields, e.g., /PN, <<<  
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<  
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<  
>>> enter this cluster. <<<  
>>> <<<  
>>> Use USPATALL when searching terms such as patent assignees, <<<  
>>> classifications, or claims, that may potentially change from <<<

&gt;&gt;&gt; the earliest to the latest publication.

&lt;&lt;&lt;

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

L3 STR  
L7 16 SEA FILE=REGISTRY SSS FUL L3  
L9 16 SEA FILE=USPATFULL ABB=ON L7

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FILE 'CAPLUS' ENTERED AT 16:13:19 ON 27 FEB 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE 'USPATFULL' ENTERED AT 16:13:19 ON 27 FEB 2004  
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)  
PROCESSING COMPLETED FOR L8  
PROCESSING COMPLETED FOR L9

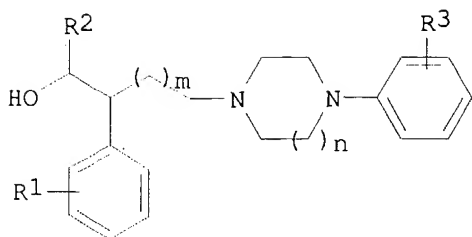
L11 31 DUP REM L8 L9 (0 DUPLICATES REMOVED)  
ANSWERS '1-15' FROM FILE CAPLUS  
ANSWERS '16-31' FROM FILE USPATFULL

=&gt; d ibib ed abs hitstr l11 1-31; fil cao; d que nos l10

L11 ANSWER 1 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2003:1006971 CAPLUS  
DOCUMENT NUMBER: 140:59660  
TITLE: Preparation of disubstituted diazacycloalkanes as  
serotonin 5-HT1A ligands for treatment of  
neuromuscular dysfunction of the lower urinary tract.  
INVENTOR(S): Leonardi, Amedeo; Motta, Gianni; Riva, Carlo; Testa,  
Rodolfo  
PATENT ASSIGNEE(S): Recordati S.A., Switz.; Recordati Industria Chimica e  
Farmaceutica S.p.A.  
SOURCE: PCT Int. Appl., 54 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003106444	A1	20031224	WO 2003-EP6280	20030616
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, FR, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: IT 2002-MI1328 A 20020614  
OTHER SOURCE(S): MARPAT 140:59660  
ED Entered STN: 26 Dec 2003  
GI



I

AB Title compds. I; [R1 = halo; R2 = C3-8 cycloalkyl; R3 = C1-4 alkoxy, haloalkoxy; m, n = 1, 2], were prepd. for treatment of urinary urgency, overactive bladder, increased urinary frequency, decreased urinary compliance (decreased bladder storage capacity), cystitis (including interstitial cystitis), incontinence, urine leakage, enuresis, dysuria, urinary hesitancy and difficulty in emptying the bladder. I and their enantiomers, diastereoisomers, N-oxides, polymorphs, solvates and pharmaceutically acceptable salts are useful in the treatment of patients with neuromuscular dysfunction of the lower urinary tract and diseases related to 5-HT1A receptor. Thus, 4-cyclohexyl-4-oxo-3-(2-fluorophenyl)butyraldehyde (prepn. given), 1-(2-methoxyphenyl)piperazine HCl, Na triacetoxyborohydride and CH2Cl2 were stirred together at r.t. for 1 h and kept overnight to give 1-[4-cyclohexyl-4-oxo-3-(2-fluorophenyl)butyl]-4-(2-methoxyphenyl)piperazine. The latter was stirred with NaBH4 in MeOH to give (SR,RS)- and (RR,SS)-1-cyclohexyl-4-[4-(2-methoxyphenyl)piperazin-1-yl]-2-(2-fluorophenyl)butan-1-ol. The (SR,RS)-diastereomer bound to 5-HT1A receptors with Ki = 0.13 nM.

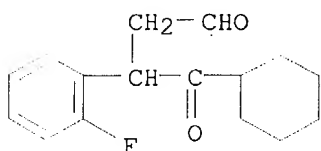
IT 636598-27-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of hydroxyalkyldiazacycloalkanes as serotonin ligands for treatment of neuromuscular dysfunction of the lower urinary tract)

RN 636598-27-1 CAPLUS

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-2-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:1006970 CAPLUS

DOCUMENT NUMBER: 140:42211

TITLE: Preparation of phenylalkylpiperazines for treatment of diseases related to 5-HT1A receptor activity.

INVENTOR(S): Leonardi, Amadeo; Motta, Gianni; Riva, Carlo; Poggesi, Elena

PATENT ASSIGNEE(S): Recordati S.A. Switz.; Recordati Industria Chimica e Farmaceutica S.p.A.

SOURCE: PCT Int. Appl. 106 pp.

CODEN: PTXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

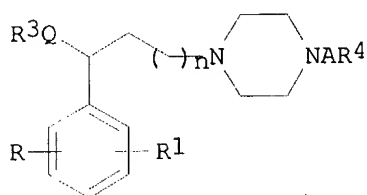
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WO 2003106443	A1	20031224	WO 2003-EP6289	20030616
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: IT 2002-MI1327 A 20020614

OTHER SOURCE(S): MARPAT 140:42211

ED Entered STN: 26 Dec 2003

GI



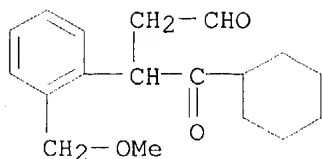
AB Title compds. [I; R = H, halo, alkyl, alkoxy, alkylthio, OH, alkenyl, alkynyl, haloalkyl, aminoalkyl, cyano, alkylsulfonyl, dialkylaminosulfonyl, etc.; R1 = H, (R-substituted) cycloalkyl, aryl, aryloxy, aralkyl, aralkoxy, heterocyclyl, heterocyclyloxy, heterocycloalkyl, heterocycloalkoxy; Q = CO, CH(OH), CH(OR2); R2 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R3 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl; R4 = (R-substituted) aryl, heterocyclyl; n = 1, 2; A = bond, CH2, CH2CH2], were prepd. for treatment of CNS disorders, for reducing the frequency of bladder contractions, and for treating neuromuscular dysfunction of the lower urinary tract. Thus, 4-cyclohexyl-3-(2-fluorophenyl)-4-methoxybutyraldehyde (prepn. given), 1-[2-(2,2,2-trifluoroethoxy)phenyl]piperazine hydrochloride, Na triacetoxyborohydride, AcOH and CH2Cl2 were stirred together at room temp. for 1h, and kept overnight to give 1-[4-cyclohexyl-3-(2-fluorophenyl)-4-methoxybutyl]-4-[2-(2,2,2-trifluoroethoxy)phenyl]piperazine. The latter bound to 5-HT1A receptors with Ki = 1.45 nM.

IT 636598-41-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of phenylalkylpiperazines for treatment of diseases related to 5-HT1A receptor activity)

RN 636598-41-9 CAPLUS

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-2-(methoxymethyl)- (9CI) (CA INDEX NAME)



IT 636598-06-6P 636598-22-6P 636598-26-0P

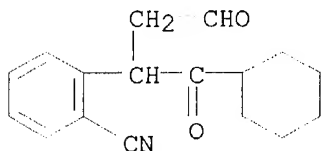
636598-27-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of phenylalkylpiperazines for treatment of diseases related to 5-HT1A receptor activity)

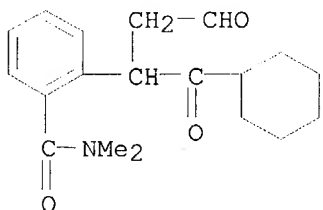
RN 636598-06-6 CAPLUS

CN Benzonitrile, 2-[1-(cyclohexylcarbonyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)



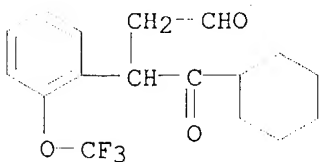
RN 636598-22-6 CAPLUS

CN Benzamide, 2-[1-(cyclohexylcarbonyl)-3-oxopropyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 636598-26-0 CAPLUS

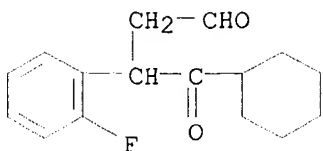
CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-2-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



RN 636598-27-1 CAPLUS

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-2-fluoro- (9CI) (CA INDEX NAME)



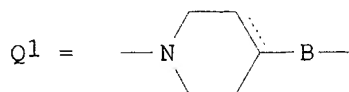
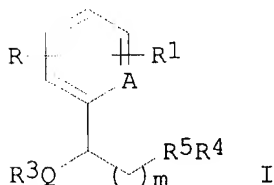


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2003:1006953 CAPLUS  
 DOCUMENT NUMBER: 140:59523  
 TITLE: Preparation of phenylalkylamines and pyridylalkylamines as 5-HT1A serotonergic ligands.  
 INVENTOR(S): Leonardi, Amedeo; Motta, Gianni; Riva, Carlo; Guarneri, Luciano  
 PATENT ASSIGNEE(S): Recordati S.A., Switz.; Recordati Industria Chimica e Farmaceutica S.p.A.  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003106421	A2	20031224	WO 2003-EP6290	20030616
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: IT 2002-MI1329 A 20020614  
 OTHER SOURCE(S): MARPAT 140:59523  
 ED Entered STN: 26 Dec 2003  
 GI



AB Title compds. [I; R = H, halo, alkyl, alkoxy, alkylthio, OH, halo, alkenyl, alkynyl, alkylcarbonyl, alkylsulfinyl, alkylsulfonyl, dialkylaminosulfonyl, etc.; R1 = H, (substituted) cycloalkyl, aryl, aryloxy, aralkyl, aralkoxy, heterocyclyl, heterocycloalkyl, heterocycloxy, heterocycloalkoxy; Q = CO, CH(OH), CH(OR2); R2 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R3 = (substituted)

alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl; R4 = (substituted) aryl, heterocyclyl; A = CH, N; R5 = NR6(CH2)nR7, Q1; m, n = 2, 3; R6 = H, alkyl; R7 = O, S, NR6, CH2; B = bond, O, S, NR6, CH2; dotted line = optional double bond; with provisos], were prepd. for treatment of neuromuscular dysfunction of the lower urinary tract (no data). Thus, 3-(2-cyanophenyl)-4-cyclohexyl-4-oxobutyraldehyde (prepn. given), 8-(N-methyl-2-aminoethoxy)quinoline, and Na(AcO)3BH were stirred with AcOH in CH2Cl2 for 1 h to give 52% 8-[N-[3-(2-cyanophenyl)-4-cyclohexyl-4-oxobutyl]-N-methyl-2-aminoethoxy]quinoline.

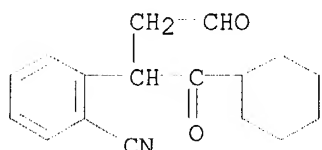
IT 636598-06-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of phenylalkylamines and pyridylalkylamines as 5-HT1A serotonergic ligands)

RN 636598-06-6 CAPLUS

CN Benzonitrile, 2-[1-(cyclohexylcarbonyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)



L11 ANSWER 4 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:51440 CAPLUS

DOCUMENT NUMBER: 136:102392

TITLE: Preparation of phenylpyridazine derivatives as inhibitors of interleukin-1-beta. production

INVENTOR(S): Ohkuchi, Masao; Kyotani, Yoshinori; Shigyo, Hiromichi; Koshi, Tomoyuki; Ohgiya, Tadaaki; Matsuda, Takayuki; Kumai, Natsuyo; Yasuoka, Kyoko

PATENT ASSIGNEE(S): Kowa Co., Ltd., Japan

SOURCE: PCT Int. Appl., 70 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

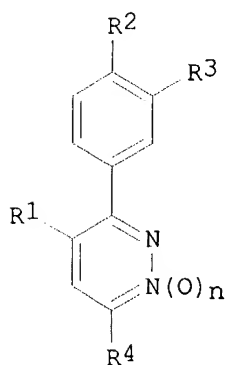
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004427	A1	20020117	WO 2001-JP5904	20010706
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US 6664256	B1	20031216	US 2000-612953	20000710
AU 2001069474	A5	20020121	AU 2001-69474	20010706
EP 1300399	A1	20030409	EP 2001-947902	20010706
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
NO 2003000097	A	20030109	NO 2003-97	20030109
PRIORITY APPLN. INFO.: US 2000-612953 A 20000710				
WO 2001-JP5904 W 20010706				

OTHER SOURCE(S): MARPAT 136:102392  
 ED Entered STN: 18 Jan 2002  
 GI



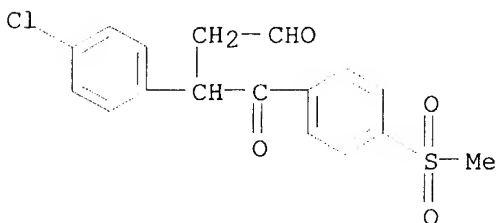
AB Compds. of the general formula (I) or salts thereof [wherein R1 is optionally substituted Ph or pyridyl; R2 is lower alkoxy, lower alkylthio, lower alkylsulfinyl, or lower alkylsulfonyl; R3 is hydrogen or lower alkoxy; or R2 and R3 together form a alkylenedioxy group; and R4 is hydrogen, halo, cyano, CO<sub>2</sub>H, each optionally substituted lower alkyl, lower alkenyl, lower alkylthio, lower alkylsulfinyl, lower alkylsulfonyl, lower alkylsulfonyloxy, arom. hydrocarbonyl, arom. heterocyclyl, phenoxy, phenylthio, phenylsulfinyl, phenylsulfonyl, pyridyloxy, morpholino, morpholinocarbonyl, piperidinocarbonyl, 1-piperazinylcarbonyl, or NH<sub>2</sub>; n = 0, 1] are prepd. The compds. I exhibit an excellent interleukin 1.β. prodn. inhibiting activity and are useful as preventive and therapeutic drugs for diseases caused by increased prodn. of interleukin 1.β. such as immunol. diseases, inflammatory diseases, ischemic disease, osteoporosis, septicemia, rheumatism, arthritis, and inflammatory colitis. Thus, 2,3,4,5,6-pentafluorophenol and K<sub>2</sub>CO<sub>3</sub> were added to a soln. of 6-chloro-3-(4-methoxyphenyl)-4-phenylpyridazine in DMF and stirred at 80.degree. for 7 h to give 30.5% 3-(4-methoxyphenyl)-6-(2,3,4,5,6-pentafluorophenoxy)-4-phenylpyridazine (II). II showed IC<sub>50</sub> of 0.01 .μM for inhibiting the prodn. of interleukin-1.β. in HL-60 cells.

IT **388606-95-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. of phenylpyridazine derivs. as inhibitors of interleukin 1.β. prodn. and preventive and therapeutic drugs for diseases caused by increased prodn. of interleukin 1.β.)

RN 388606-95-9 CAPLUS

CN Benzenebutanal, .β.-(4-chlorophenyl)-4-(methylsulfonyl)-.γ.-oxo-  
 (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2002:337331 CAPLUS  
DOCUMENT NUMBER: 137:78926  
TITLE: ~~Asymmetric Construction of Quaternary Centers by~~  
Enantioselective Allylation: Application to the  
Synthesis of the Serotonin Antagonist LY426965  
AUTHOR(S): Denmark, Scott E.; Fu, Jiping  
CORPORATE SOURCE: Roger Adams Laboratory, Department of Chemistry,  
University of Illinois, Urbana, IL, 61801, USA  
SOURCE: Organic Letters (2002), 4(11), 1951-1953  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 137:78926  
ED Entered STN: 07 May 2002  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Serotonin antagonist LY426965 I (R = cyclohexyl) and a related antagonist I (R = Ph) are prepd. enantioselectively in 6-8 steps from benzaldehyde, phenylacetylene, and 1-(2-methoxy)piperazine using the asym. allylation of benzaldehyde with allylic trichlorosilane (E)-PhC(Me):CHCH<sub>2</sub>SiCl<sub>3</sub> (II) in the presence of bisdipyrrolodiazaphosphole ligand III as the key step. Phenylacetylene undergoes addn. with zirconocene dichloride and trimethylaluminum followed by lithiation and hydroxymethylation to provide (E)-PhC(Me):CHCH<sub>2</sub>OH; chlorination of the allylic alc. with NCS and substitution of the chloride with trichlorosilane gives II. In the key step, addn. of benzaldehyde to a soln. of II in the presence of III and tetrabutylammonium iodide gives the homoallylic alc. IV in 91% yield, 98% de, and 94% er. Hydroboration of IV, selective hydrogenation of the Ph moiety alpha to the secondary alc., Swern oxidn. of both alcs., and reductive amination of the aldehyde moiety with 1-(2-methoxyphenyl)piperazine gives I (R = cyclohexyl). Swern oxidn. of IV followed by reductive amination of the aldehyde moiety with 1-(2-methoxyphenyl)piperazine gives I (R = Ph). The preps. of I (R = cyclohexyl, Ph) illustrate the ability of the asym. Lewis base-catalyzed allylation of aldehydes with allylic trichlorosilanes to set quaternary carbon centers with good stereoselectivity and to provide functionalized mols. contg. quaternary carbon stereocenters.

IT 440369-03-9P

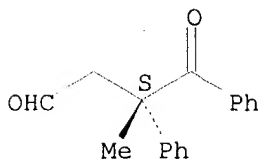
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(asym. prepn. of a serotonin antagonist using the Lewis base-catalyzed asym. allylation of aldehydes with allylic trichlorosilanes to set a quaternary carbon stereocenter in the key step)

RN 440369-03-9 CAPLUS

CN Benzenebutanal, .beta.-methyl-.gamma.-oxo-.beta.-phenyl-, (.beta.S)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 440369-06-2P

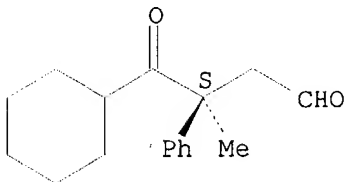
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(asym. prepn. of the serotonin antagonist LY426965 using the Lewis base-catalyzed asym. allylation of aldehydes with allylic trichlorosilanes to set a quaternary carbon stereocenter in the key step)

RN 440369-06-2 CAPLUS

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl-, (.beta.S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:730724 CAPLUS

DOCUMENT NUMBER: 135:272860

TITLE: Enantioselective process for preparing arylated lactones and derivatives

INVENTOR(S): Zhang, Tony Yantao; Zhang, Hongbin; Proctor, Christophor Scott

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001072731	A2	20011004	WO 2001-US5800	20010312
WO 2001072731	A3	20030116		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1286980	A2	20030305	EP.2001-918212	20010312
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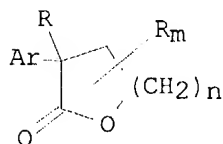
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2003225282 A1 20031204 US 2003-220444 20030318  
PRIORITY APPLN. INFO.: US 2000-192148P P 20000324  
WO 2001-US5800 W 20010312

OTHER SOURCE(S): CASREACT 135:272860; MARPAT 135:272860

ED Entered STN: 07 Oct 2001

GI



AB A process for the arylation of lactones to form to chiral and achiral aryllactones (I) having high enantioselectivity where applicable is described. These aryllactones can be used to prep. compds. chiral or achiral ketones  $R_1COC(Ar)(R)CH_2CH_2NR_2R_3$ . Thus, .alpha.-(3,4-dimethoxyphenyl)-.alpha.-methyl-.gamma.-butyrolactone was prepd. from .alpha.-methyl-.gamma.-butyrolactone and 1,2-dimethoxy-4-bromobenzene in the presence of a base  $[KN(TMS)_2]$  using  $Pd(OAc)_2/(R)-(+)-BINAP$  as the catalyst.

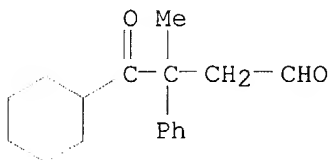
IT 228419-04-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and condensation reaction with arylpiperazine)

RN 228419-04-3 CAPLUS

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:247332 CAPLUS

DOCUMENT NUMBER: 134:280711

TITLE: Preparation of 4-(benzothienyl)piperidines as ~~serotonin reuptake inhibitors~~

INVENTOR(S): Kohlman, Daniel Timothy; Liang, Sidney Xi; Xu, Yao-chang

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023381	A1	20010405	WO 2000-US20824	20000914
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

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 HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,  
 LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,  
 SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
 YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,  
 CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

BR 2000014447 A 20020611 BR 2000-14447 20000914

JP 2003510322 T2 20030318 JP 2001-526533 20000914

PRIORITY APPLN. INFO.:

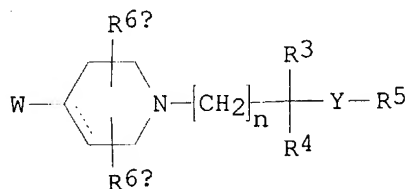
US 1999-157343P P 19990929

WO 2000-US20824 W 20000914

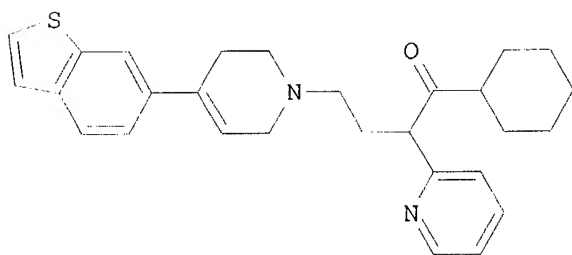
OTHER SOURCE(S): MARPAT 134:280711

ED Entered STN: 06 Apr 2001

GI



I



II

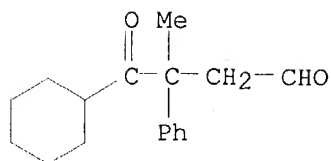
AB The title compds. [I; W = (un)substituted benzothienyl, benzofuranyl; Y = CO, CHOH, CH2, etc.; n = 1-4; R3 = O, OH, hydroxyalkyl, etc.; R4 = (un)substituted aryl, heterocyclyl, cycloalkyl; R5 = (un)substituted aryl, heterocyclyl, cycloalkyl; R6a, R6b = H, alkyl] which inhibit the reuptake of serotonin and antagonize the serotonin receptor, and therefore are useful in alleviating the symptoms caused by withdrawal or partial withdrawal from the use of tobacco or of nicotine, and treating depression, were prepd. and formulated. E.g., a multi-step synthesis of II was given.

IT 228419-04-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. of 4-(benzothienyl)piperidines as serotonin reuptake inhibitors)

RN 228419-04-3 CAPLUS

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)

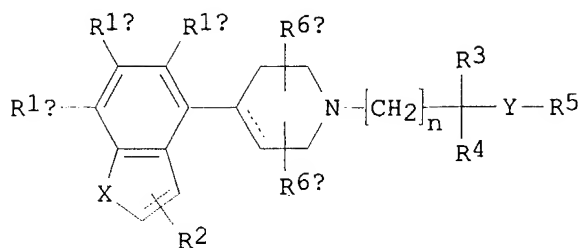


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

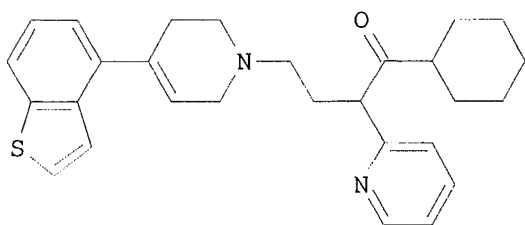
L11 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2001:247331 CAPLUS  
DOCUMENT NUMBER: 134:280710  
TITLE: Preparation of benzothienyl-substituted piperidines as serotonin reuptake inhibitors  
INVENTOR(S): Liang, Sidney Xi; Xu, Yao-chang  
PATENT ASSIGNEE(S): Eli Lilly and Company, USA  
SOURCE: PCT Int. Appl., 85 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023380	A1	20010405	WO 2000-US20823	20000914
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000014668	A	20020618	BR 2000-14668	20000914
EP 1220853	A1	20020710	EP 2000-961329	20000914
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003510321	T2	20030318	JP 2001-526532	20000914
US 6664274	B1	20031216	US 2002-70183	20020716
PRIORITY APPLN. INFO.:			US 1999-156762P	P 19990929
			WO 2000-US20823	W 20000914
OTHER SOURCE(S):		MARPAT 134:280710		
ED Entered STN:		06 Apr 2001		
GI				





I



II

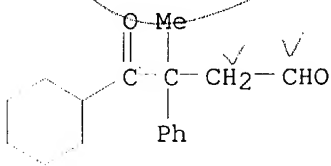
AB The title compds. [I; X = O, S; Y = CO, CHOH, CH<sub>2</sub>, etc.; n = 1-4; R1a, R1b, R1c, R2 = H, F, Cl, etc.; R3 = H, OH, hydroxyalkyl, etc.; R4 = aryl, heterocyclyl, cycloalkyl, etc.; R5 = aryl, heterocyclyl, cycloalkyl, etc.; R6a, R6b = H, alkyl] which inhibit the reuptake of serotonin, antagonize the 5-HT1A receptor and antagonize the 5-HT2A receptor, and therefore are useful for alleviating the symptoms caused by withdrawal from the use of tobacco or nicotine, and depression, were prepd. and formulated. E.g., a multi-step synthesis of II was given.

IT 228419-04-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of benzothienyl-substituted piperidines as serotonin reuptake inhibitors)

RN 228419-04-3 CAPLUS

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:15021 CAPLUS

DOCUMENT NUMBER: 132:64187

TITLE: Preparation of azepine derivatives having effects on serotonin related systems

INVENTOR(S): Hauser, Kenneth Lee; Hertel, Larry Wayne; Xu, Yao-Chang

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 112 pp.

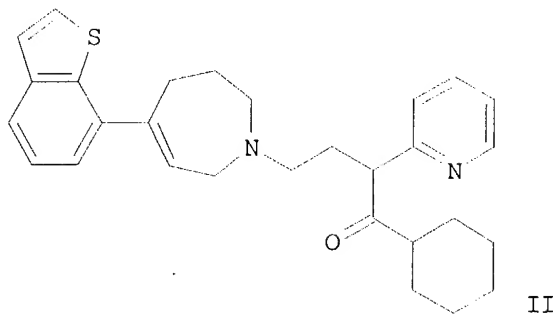
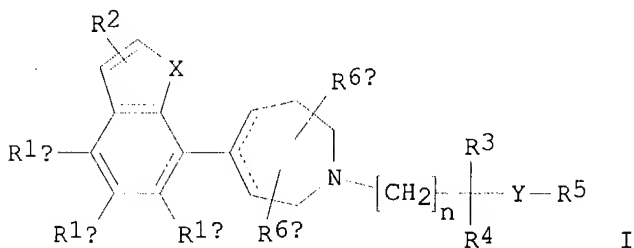
CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000000203	A1	20000106	WO 1999-US14778	19990629
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2335310	AA	20000106	CA 1999-2335310	19990629
AU 9947277	A1	20000117	AU 1999-47277	19990629
EP 1091741	A1	20010418	EP 1999-930830	19990629
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
JP 2002519326	T2	20020702	JP 2000-556788	19990629
US 6465453	B1	20021015	US 2000-701363	20001128
US 2002193590	A1	20021219	US 2002-141424	20020508
PRIORITY APPLN. INFO.:			US 1998-91245P	P 19980630
			WO 1999-US14778	W 19990629
			US 2000-701363	A3 20001128
OTHER SOURCE(S):			MARPAT 132:64187	
ED Entered STN: 07 Jan 2000				
GI				



AB The title compds. [I; X = O, S, NR, SO, SO<sub>2</sub>; Y = CO, CH(OH), CH<sub>2</sub>, etc.; n = 1-4; R = H, alkyl; R<sub>1a</sub>, R<sub>1b</sub>, R<sub>1c</sub>, R<sub>2</sub> = H, F, Cl, etc.; R<sub>3</sub> = H, OH,

alkyl, etc.; R4 = (un)substituted aryl, heterocyclyl, cycloalkyl; R5 = (un)substituted aryl, heterocyclyl, cycloalkyl; R6a, R6b = H, alkyl], useful in inhibiting the reuptake of serotonin, antagonizing the 5-HT1A receptor and antagonizing the 5-HT2A receptor, and therefore useful in treating depression, were prepd. and formulated. E.g., a multi-step synthesis of the title compd. II was given. Compds. I are effective at 20-25 mg/day.

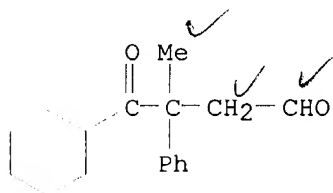
IT 228419-04-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of azepine derivs. having effects on serotonin related systems)

RN 228419-04-3 CAPLUS

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:15012 CAPLUS

DOCUMENT NUMBER: 132:64175

TITLE: Preparation of piperidine derivatives having effects on serotonin related systems

INVENTOR(S): Hertel, Larry Wayne; Kohlmam, Daniel Timothy; Liang, Sidney Xi; Wong, David Taiwai; Xu, Yao-Chang

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 143 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

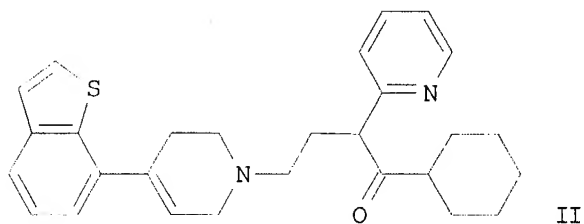
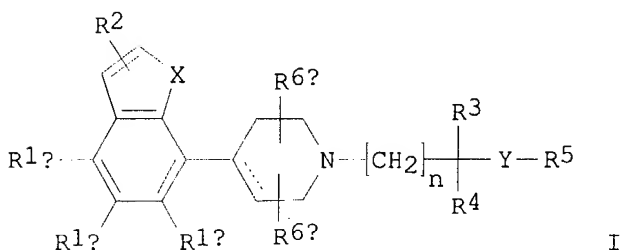
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000000198	A1	20000106	WO 1999-US14732	19990629
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2336117	AA	20000106	CA 1999-2336117	19990629
AU 9947266	A1	20000117	AU 1999-47266	19990629
EP 982304	A1	20000301	EP 1999-305095	19990629
EP 982304	B1	20021002		
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EP 1146045	A1	20011017	EP 2001-202620	19990629
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				

JP 2002519323	T2	20020702	JP 2000-556783	19990629
AT 225345	E	20021015	AT 1999-305095	19990629
ES 2181366	T3	20030216	ES 1999-305095	19990629
US 6436964	B1	20020820	US 2000-701406	20001128
PRIORITY APPLN. INFO.:			US 1998-91241P	P 19980630
			EP 1999-305095	A3 19990629
			WO 1999-US14732	W 19990629

OTHER SOURCE(S): MARPAT 132:64175

ED Entered STN: 07 Jan 2000

GI



AB The title compds. [I; X = O, S, SO, SO<sub>2</sub>, NR; Y = CO, CH(OH), CH<sub>2</sub>, etc.; n = 1-4; R = H, alkyl; R1a, R1b, R1c, R2 = H, F, Cl, Br, etc.; R3 = O, OH, alkyl, etc.; R4 = (un)substituted aryl, heterocyclyl, cycloalkyl, etc., R5 = (un)substituted aryl, heterocyclyl, cycloalkyl, etc., R6a, R6b = H, alkyl] and their pharmaceutically acceptable salts, useful for inhibiting the reuptake of serotonin, antagonizing the 5-HT<sub>1A</sub> receptor and antagonizing the 5-HT<sub>2A</sub> receptor, and therefore useful in treating depression, were prepd. and formulated. E.g., a multi-step synthesis of tetrahydropyridine II.oxalate, was given. In general, compds. I are effective at 1-200 mg/day.

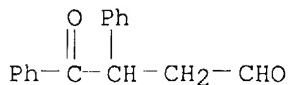
IT 147031-23-0P 228419-04-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of piperidine derivs. having effects on serotonin related systems)

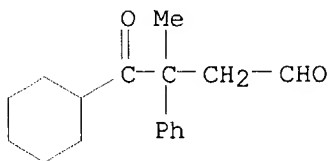
RN 147031-23-0 CAPLUS

CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-04-3 CAPLUS

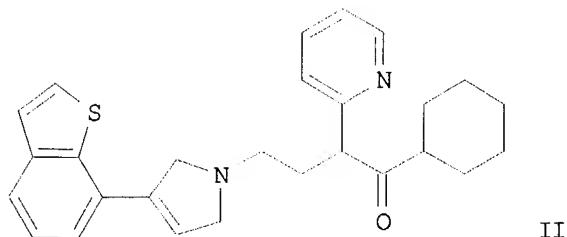
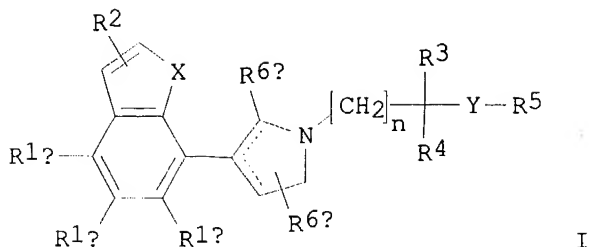
CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA  
INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2000:15008 CAPLUS  
DOCUMENT NUMBER: 132:78467  
TITLE: Preparation of pyrrolidine and pyrroline derivatives  
having effects on serotonin related systems  
INVENTOR(S): Hertel, Larry Wayne; Xu, Yao-chang  
PATENT ASSIGNEE(S): Eli Lilly and Company, USA  
SOURCE: PCT Int. Appl., 113 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000000196	A1	20000106	WO 1999-US14881	19990629
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2334897	AA	20000106	CA 1999-2334897	19990629
AU 9948501	A1	20000117	AU 1999-48501	19990629
EP 1100501	A1	20010523	EP 1999-932127	19990629
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
JP 2002519321	T2	20020702	JP 2000-556781	19990629
US 6353008	B1	20020305	US 2000-701361	20001128
PRIORITY APPLN. INFO.: US 1998-91204P P 19980630 WO 1999-US14881 W 19990629				
OTHER SOURCE(S): MARPAT 132:78467				
ED Entered STN: 07 Jan 2000				
GI				



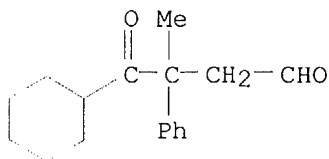
AB The title compds. [I; X = O, S, NR, SO, SO<sub>2</sub>; Y = CO, CH(OH), CH<sub>2</sub>, etc.; n = 1-4; R = H, alkyl; R1a, R1b, R1c, R2 = H, F, Cl, etc.; R3 = H, OH, alkyl, etc.; R4 = (un)substituted aryl, heterocyclyl, cycloalkyl; R5 = (un)substituted aryl, heterocyclyl, cycloalkyl; R6a, R6b = H, alkyl] which inhibit the reuptake of serotonin, antagonize the 5-HT<sub>1A</sub> receptor and antagonize the 5-HT<sub>2A</sub> receptor, and therefore are useful in the treatment of depression, were prepd. and formulated. Thus, treatment of 3-(2-pyridyl)-4-cyclohexyl-4-keto-butyraldehyde ethylene ketal with 3N HCl followed by addn. of Na<sub>2</sub>SO<sub>4</sub> and 3,4-dihydro-3-(7-benzothiophenyl)pyrrolidine in CH<sub>2</sub>Cl<sub>2</sub>, and then NaBH(OAc)<sub>3</sub> afforded 24% II. Compds. I are effective, in general, at 1-200 mg/day.

IT **228419-04-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of pyrrolidine and pyrroline derivs. having effects on serotonin related systems)

RN 228419-04-3 CAPLUS

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:401578 CAPLUS

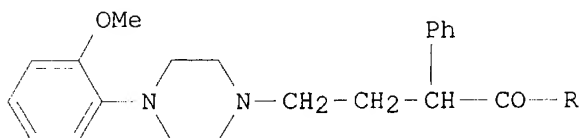
DOCUMENT NUMBER: 131:58847

TITLE: Arylpiperazines having activity at the serotonin 1a receptor

INVENTOR(S): Kohlman, Timothy Daniel; Xu, Yao-chang; Godfrey, Alexander Glenn; O'Toole, John Cunningham; Zhang, Tony

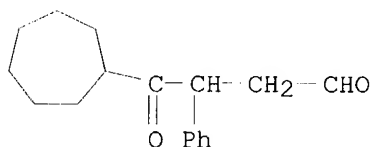
PATENT ASSIGNEE(S): Yantao  
 SOURCE: Eli Lilly and Co., USA  
 Eur. Pat. Appl., 47 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 924205	A1	19990623	EP 1998-310223	19981214
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TW 520366	B	20030211	TW 1998-87119922	19981201
CA 2315227	AA	19990624	CA 1998-2315227	19981208
WO 9931077	A1	19990624	WO 1998-US26008	19981208
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9918083	A1	19990705	AU 1999-18083	19981208
AU 747040	B2	20020509		
BR 9814280	A	20011030	BR 1998-14280	19981208
JP 2002508364	T2	20020319	JP 2000-539004	19981208
NZ 505220	A	20021126	NZ 1998-505220	19981208
US <del>6239135</del>	B1	20010529	US 1998-208553	19981209
ZA 9811473	A	20000614	ZA 1998-11473	19981214
NO 2000003082	A	20000802	NO 2000-3082	20000615
HR 2000000406	A1	20001231	HR 2000-406	20000616
US 2001003749	A1	20010614	US 2001-753645	20010103
US <del>6358958</del>	B2	20020319		
US 2002169170	A1	20021114	US 2001-22045	20011218
US <del>6645967</del>	B2	20031111		
US 2003027831	A1	20030206	US 2001-22043	20011218
US <del>6660859</del>	B2	20031209		
AU 761622	B2	20030605	AU 2002-27468	20020320
AU 2002027468	A5	20020509		
US 2003008879	A1	20030109	US 2002-136101	20020430
US <del>6514976</del>	B2	20030204		
PRIORITY APPLN. INFO.:			US 1997-69722P	P 19971216
			US 1997-69791P	P 19971216
			US 1998-89589P	P 19980617
			AU 1999-18083	A3 19981208
			WO 1998-US26008	W 19981208
			US 1998-208553	A3 19981209
			US 2001-753645	A3 20010103
			US 2001-22043	A3 20011218
OTHER SOURCE(S):			MARPAT 131:58847	
ED Entered STN: 30 Jun 1999				
GI				

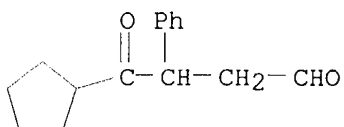


AB Aryl piperazine compds. are effective pharmaceuticals for the treatment of conditions related to or affected by the serotonin 1A receptor; the compds. are particularly effective antagonists at that receptor, and are particularly useful for alleviating the symptoms of nicotine and tobacco withdrawal. Title compds. such as I (R = Ph, cyclohexyl, cycloheptyl, cyclopentyl) were prepd. from 1-(2-methoxyphenyl)piperazine and RCOCHPhCH<sub>2</sub>CHO in 67-95% yields. Among the approx. 5 other compds. similarly prepd. were 1-(2-methoxyphenyl)-4-[3-cyclohexanecarbonyl-3-(phenyl)butyl]piperazine, 1-(2-pyridyl)-4-[3-cyclohexanecarbonyl-3-(phenyl)butyl]piperazine and 1-(2-ethoxyphenyl)-4-[3-cyclohexanecarbonyl-3-(phenyl)butyl]piperazine.

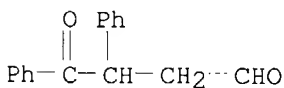
IT 228419-09-8, 3-Cycloheptanecarbonyl-3-phenylpropanal  
 228419-10-1, 3-Cyclopentanecarbonyl-3-phenylpropanal  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of arylpiperazines having activity at serotonin 1a receptor)  
 RN 228419-09-8 CAPLUS  
 CN Cycloheptanebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-10-1 CAPLUS  
 CN Benzenepropanal, .beta.-(cyclopentylcarbonyl)- (9CI) (CA INDEX NAME)

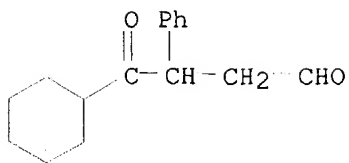


IT 147031-23-0P, 3-Benzoyl-3-phenylpropionaldehyde  
 228418-97-1P, 3-Cyclohexanecarbonyl-3-propanal  
 228419-00-9P, 3-Benzoyl-3-phenylbutanal 228419-04-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. of arylpiperazines having activity at serotonin 1a receptor)  
 RN 147031-23-0 CAPLUS  
 CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)

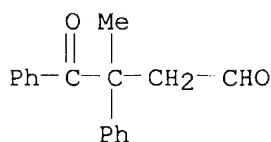


RN 228418-97-1 CAPLUS  
 CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)- (9CI) (CA INDEX NAME)

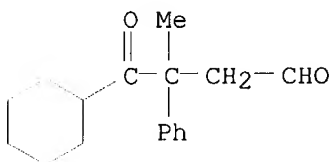




RN 228419-00-9 CAPLUS  
 CN Benzenebutanal, .beta.-methyl-.gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)

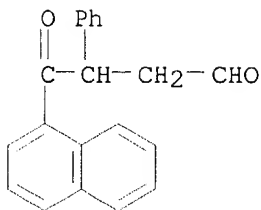


RN 228419-04-3 CAPLUS  
 CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

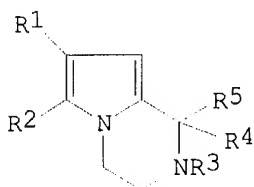
L11 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1999:800854 CAPLUS  
 DOCUMENT NUMBER: 132:122504  
 TITLE: 1,3,4,5-Tetrahydroazepin-2-ones by dearomatising anionic cyclisation of N-allyl-1-naphthamides  
 AUTHOR(S): Ahmed, Anjum; Clayden, Jonathan; Rowley, Michael  
 CORPORATE SOURCE: Dep. Chemistry, Univ. Manchester, Manchester, M13 9PL, UK  
 SOURCE: Synlett (1999), (12), 1954-1956  
 CODEN: SYNLES; ISSN: 0936-5214  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 132:122504  
 ED Entered STN: 20 Dec 1999  
 AB On treatment with Me3CLi and DMPU, 1-naphthamides bearing N-allyl or N-prenyl substituents cyclize to give a mixt. of products from which 7-membered lactams were isolated in .ltoreq.73% yield.  
 IT **256418-40-3P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of hydroazepinones by dearomatizing anionic cyclization of N-allylnaphthamides)  
 RN 256418-40-3 CAPLUS  
 CN 1-Naphthalenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



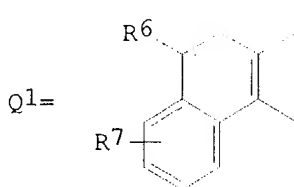
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1993:234081 CAPLUS  
DOCUMENT NUMBER: 118:234081  
TITLE: Preparation of pyrrolo[1,2-.alpha.]pyrazines and benzo[g]pyrazinoindoles as monoamine oxidase inhibitors  
INVENTOR(S): Roever, Stephan  
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.  
SOURCE: Eur. Pat. Appl., 53 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 521368	A1	19930107	EP 1992-110531	19920623
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, PT, SE				
ZA 9204720	A	19930331	ZA 1992-4720	19920625
<u>US 5292732</u>	A	19940308	US 1992-905584	19920626
HU 70163	A2	19950928	HU 1992-2139	19920626
IL 102337	A1	19960131	IL 1992-102337	19920626
AU 9219309	A1	19930107	AU 1992-19309	19920629
AU 654362	B2	19941103		
CA 2072836	AA	19930103	CA 1992-2072836	19920630
NO 9202604	A	19930104	NO 1992-2604	19920701
BR 9202558	A	19930316	BR 1992-2558	19920701
CN 1068328	A	19930127	CN 1992-105314	19920702
CN 1030986	B	19960214		
JP 06239865	A2	19940830	JP 1992-197449	19920702
JP 07074217	B4	19950809		
PRIORITY APPLN. INFO.:			CH 1991-1950	19910702
			CH 1992-1667	19920522
OTHER SOURCE(S):		MARPAT 118:234081		
ED Entered STN: 12 Jun 1993				
GI				



I



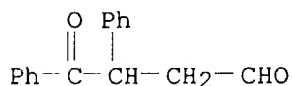
AB Title compds. [I; one of R1, R2 = aryl, the other = H, alkyl, aryl; R1R2 = Q1; R3 = H, alkyl; R4 = H; R3R4 = bond; R5, R6 = H, alkyl; R7 = H, halo, alkyl, (substituted) alkoxy, cycloalkyl, cycloalkenyl, cycloalkoxy, OH, F3CSO2O, (substituted) PhCH2O2CO; dotted line = optional double bond], were prepd. Thus, a suspension of Rieke Mg in THF was treated sequentially with 2-(2-bromoethyl)-1,3-dioxolone, CuI, and 3-ClC6H4COC1 to give 3'-chloro-3-(1,3-dioxolon-2-yl)propionophenone. This was treated with 2N HCl in THF to give a residue which was stirred with AcNHCH2CH2NH2 in HOAc to give N-[2-[2-(m-chlorophenyl)pyrrol-1-yl]ethyl]acetamide. This was refluxed in POCl3 to give, after salification, 6-(m-chlorophenyl)-3,4-dihydro-1-methylpyrrolo[12-a]pyrazine fumarate. I inhibited monoamine oxidase activity on 5-hydroxytryptamine in rat brain homogenate with IC50 = 0.0008-0.3 .mu.M. Pharmaceutical I formulations are given.

IT 147031-23-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for pyrrolopyrazine deriv. monoamine  
oxidase inhibitor)

RN 147031-23-0 CAPLUS

CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 15 OF 31 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1968:486763 CAPLUS

DOCUMENT NUMBER: 69:86763

TITLE: Reaction of 4-benzopyrones with dimethylsulfoxonium  
methylide

AUTHOR(S): Caplin, G. A.; Ollis, W. D.; Sutherland, I. O.

CORPORATE SOURCE: Univ. Sheffield, Sheffield, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic  
(1968), (18), 2302-10

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 69:86763

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

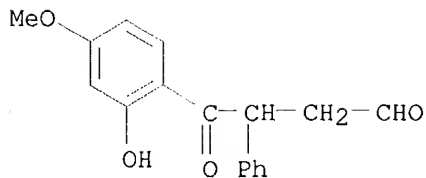
AB The reaction of 4-benzopyrones with Me2S+OCH2 gives three types of products: 2,3-dihydro-2,3-methano-4-benzopyrones (I), 2-vinylcoumaran-3-ones, and 1-(2-hydroxyaryl)butane-1,4-diones (II). I are readily hydrolyzed to II; and this reaction may occur during the isolation of the latter products. The structural relation between these products is discussed in terms of reaction mechanism, and the effects of substituents upon product ratios are also considered.

IT 19725-66-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 19725-66-7 CAPLUS

CN Hydrocinnamaldehyde, .beta.-(2-hydroxy-p-anisoyl)- (8CI) (CA INDEX NAME)



L11 ANSWER 16 OF 31 USPATFULL on STN

ACCESSION NUMBER: 2003:319533 USPATFULL

TITLE: Enantioselective process for preparing arylated lactones and derivatives

INVENTOR(S): Zhang, Tony Yantao, Indianapolis, IN, UNITED STATES  
Zhang, Hongbin, Kunming, CHINA  
Proctor, Christophor Scott, Indianapolis, IN, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2003225282	A1	20031204
APPLICATION INFO.:	US 2003-220444	A1	20030318 (10)
	WO 2001-US5800		20010312
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	ELI LILLY AND COMPANY, PATENT DIVISION, P.O. BOX 6288, INDIANAPOLIS, IN, 46206-6288		
NUMBER OF CLAIMS:	20		
EXEMPLARY CLAIM:	1		
LINE COUNT:	702		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention provides a process for the arylation of lactones to form to chiral and achiral aryllactones having high enantioselectivity where applicable.

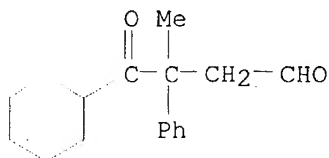
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 228419-04-3P

(prepn. and condensation reaction with arylpiperazine)

RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 17 OF 31 USPATFULL on STN

ACCESSION NUMBER: 2003:38184 USPATFULL

TITLE: Arylpiperazines having activity at the serotonin 1A receptor

INVENTOR(S): Xu, Yao-Chang, Fishers, IN, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2003027831	A1	20030206
	US 6660859	B2	20031209

APPLICATION INFO.: US 2001-22043 A1 20011218 (10)  
 RELATED APPLN. INFO.: Division of Ser. No. US 2001-753645, filed on 3 Jan 2001, GRANTED, Pat. No. US 6358958 Division of Ser. No. US 1998-208553, filed on 9 Dec 1998, GRANTED, Pat. No. US 6239135

	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-89589P	19980617 (60)
	US 1997-69722P	19971216 (60)
	US 1997-69791P	19971216 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ELI LILLY AND COMPANY, PATENT DIVISION, P.O. BOX 6288, INDIANAPOLIS, IN, 46206-6288	
NUMBER OF CLAIMS:	2	
EXEMPLARY CLAIM:	59	
LINE COUNT:	1946	
CAS INDEXING IS AVAILABLE FOR THIS PATENT.		
AB	A series of aryl piperazine compounds of the formula: ##STR1##	

wherein

Ar' is a mono or bicyclic aryl or heteroaryl radical substituted with one to three substituents selected from the group consisting of hydrogen, (C1-C6)alkyl, (C1-C6)alkoxy, (C1-C6)alkylthio, (C2-C6)alkynyl, (C1-C6)alkylhalo, (C3-C8)cycloalkyl, (C3-C8)cycloalkenyl or halo;

R1 is hydrogen, (C1-C6)alkyl, (C1-C6)alkoxy, (C1-C6)alkylthio;

R2 is phenyl, naphthyl or (C3-C12)cycloalkyl substituted with one or two substituents selected from the group consisting of hydrogen (C1-C6)alkyl, (C1-C6)alkoxy, (C1-C6)alkylthio, (C2-C6)alkenyl, (C2-C6)alkynyl, (C1-C6)alkylhalo, (C3-C8)cycloalkyl, (C3-C8)cycloalkenyl or halo;

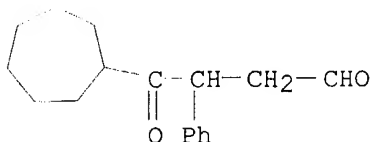
R3 is selected from the group consisting of hydrogen, (C1-C6)alkyl, (C1-C6)alkoxy, (C1-C6)alkylthio, (C2-C6)alkenyl, (C2-C6)alkynyl, (C1-C6)alkylhalo, (C3-C8)cycloalkyl, (C3-C8)cycloalkenyl or halo;

or the pharmaceutically acceptable salt, racemate, optical isomer or solvate thereof.

or the pharmaceutically acceptable salts thereof, are effective pharmaceuticals for the treatment of conditions related to or affected by the serotonin 1.sub.A receptor.

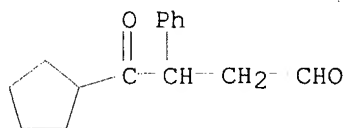
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 228419-09-8, 3-Cycloheptanecarbonyl-3-phenylpropanal  
 228419-10-1, 3-Cyclopentanecarbonyl-3-phenylpropanal  
 (prepn. of arylpiperazines having activity at serotonin 1a receptor)  
 RN 228419-09-8 USPATFULL  
 CN Cycloheptanebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)

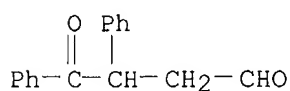


RN 228419-10-1 USPATFULL

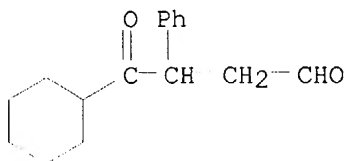
CN Benzenepropanal, .beta.-(cyclopentylcarbonyl)- (9CI) (CA INDEX NAME)



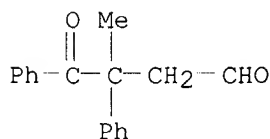
IT 147031-23-0P, 3-Benzoyl-3-phenylpropionaldehyde  
 228418-97-1P, 3-Cyclohexanecarbonyl-3-propanal  
 228419-00-9P, 3-Benzoyl-3-phenylbutanal 228419-04-3P  
 (prepn. of arylpiperazines having activity at serotonin 1a receptor)  
 RN 147031-23-0 USPATFULL  
 CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



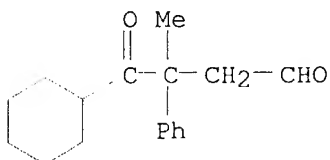
RN 228418-97-1 USPATFULL  
 CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)- (9CI) (CA INDEX NAME)



RN 228419-00-9 USPATFULL  
 CN Benzenebutanal, .beta.-methyl-.gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-04-3 USPATFULL  
 CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 18 OF 31 USPATFULL on STN  
 ACCESSION NUMBER: 2003:11175 USPATFULL

TITLE: Arylpiperazines having activity at the serotonin 1A receptor  
 INVENTOR(S): Kohlman, Daniel Timothy, Indianapolis, IN, UNITED STATES  
 Xu, Yao-Chang, Fishers, IN, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2003008879	A1	20030109
	US 6514976	B2	20030204
APPLICATION INFO.:	US 2002-136101	A1	20020430 (10)
RELATED APPLN. INFO.:	Division of Ser. No. US 2001-22043, filed on 18 Dec 2001, PENDING Division of Ser. No. US 2001-753645, filed on 3 Jan 2001, GRANTED, Pat. No. US 6358958		
	Division of Ser. No. US 1998-208553, filed on 9 Dec 1998, GRANTED, Pat. No. US 6239135		

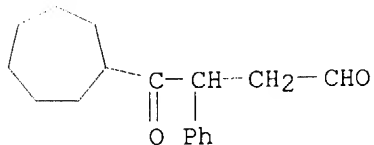
	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-89589P	19980617 (60)
	US 1997-69722P	19971216 (60)
	US 1997-69791P	19971216 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ELI LILLY AND COMPANY, PATENT DIVISION, P.O. BOX 6288, INDIANAPOLIS, IN, 46206-6288	
NUMBER OF CLAIMS:	45	
EXEMPLARY CLAIM:	1	
LINE COUNT:	2234	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

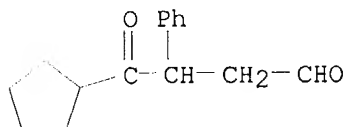
AB A series of aryl piperazine compounds are effective pharmaceuticals for the treatment of conditions related to or affected by the serotonin 1.sub.A receptor; the compounds are particularly effective antagonists at that receptor, and are particularly useful for alleviating the symptoms of nicotine and tobacco withdrawal.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 228419-09-8, 3-Cycloheptanecarbonyl-3-phenylpropanal  
 228419-10-1, 3-Cyclopentanecarbonyl-3-phenylpropanal  
 (prepn. of arylpiperazines having activity at serotonin 1a receptor)  
 RN 228419-09-8 USPATFULL  
 CN Cycloheptanebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-10-1 USPATFULL  
 CN Benzenepropanal, .beta.-(cyclopentylcarbonyl)- (9CI) (CA INDEX NAME)



IT 147031-23-0P, 3-Benzoyl-3-phenylpropionaldehyde

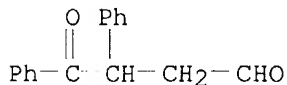
228418-97-1P, 3-Cyclohexanecarbonyl-3-propanal

228419-00-9P, 3-Benzoyl-3-phenylbutanal 228419-04-3P

(prepn. of arylpiperazines having activity at serotonin 1a receptor)

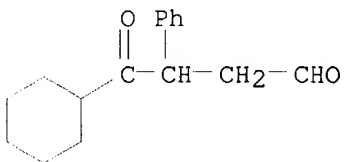
RN 147031-23-0 USPATFULL

CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



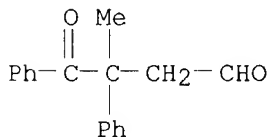
RN 228418-97-1 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)- (9CI) (CA INDEX NAME)



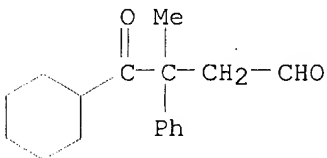
RN 228419-00-9 USPATFULL

CN Benzenebutanal, .beta.-methyl-.gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 19 OF 31 USPATFULL on STN

ACCESSION NUMBER: 2003:327013 USPATFULL

TITLE: Piperidine derivatives as serotonin reuptake inhibitors

INVENTOR(S): Liang, Sidney Xi, Hamden, CT, United States  
Xu, Yao-Chang, Fishers, IN, United States

PATENT ASSIGNEE(S): Eli Lilly and Company, Indianapolis, IN, United States  
(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6664274	B1	20031216
	WO 2001023380		20010405



APPLICATION INFO.: US 2002-70183 20020716 (10)  
WO 2000-US20823 20000914

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-156762P	19990929 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Aulakh, Charanjit S.	
LEGAL REPRESENTATIVE:	Sayles, Michael J.	
NUMBER OF CLAIMS:	17	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)	
LINE COUNT:	2387	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides compounds of formula I ##STR1##

and a method of inhibiting the reuptake of serotonin, antagonizing the 5-HT.sub.1A receptor and antagonizing the 5-HT.sub.2A receptor which comprises administering to a subject in need of such treatment an effective amount of a compound of formula I.

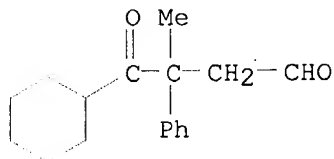
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 228419-04-3P

(prepn. of benzothienyl-substituted piperidines as serotonin reuptake inhibitors)

RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 20 OF 31 USPATFULL on STN

ACCESSION NUMBER: 2003:327009 USPATFULL

TITLE: Phenylpyridazine compounds and medicines containing the same

INVENTOR(S): Ohkuchi, Masao, Tokorogawa, JAPAN  
Kyotani, Yoshinori, Higashiyamato, JAPAN  
Shigyo, Hiromichi, Fuchu, JAPAN  
Koshi, Tomoyuki, Shiki, JAPAN  
Ohgiya, Tadaaki, Tokorozawa, JAPAN  
Matsuda, Takayuki, Higashimurayama, JAPAN  
Kumai, Natsuyo, Fujimi, JAPAN  
Kotaki, Kyoko, Sakado, JAPAN

PATENT ASSIGNEE(S): Kowa Co., Ltd., Nagoya, JAPAN (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6664256	B1	20031216
APPLICATION INFO.:	US 2000-612953		20000710 (9)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	GRANTED		
PRIMARY EXAMINER:	Bernhardt, Emily		
LEGAL REPRESENTATIVE:	Oblon, Spivak, McClelland, Maier & Neustadt, P.C.		
NUMBER OF CLAIMS:	18		

EXEMPLARY CLAIM: 1  
 NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)  
 LINE COUNT: 2057

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Phenylpyridazine compounds represented by the following formula (I):  
 ##STR1##

are provided, wherein R.sup.1, R.sup.2, R.sup.3, R.sup.4, and n are as defined herein having excellent inhibitory activity against interleukin-1.beta. production, and useful in the treatment of prevention of diseases caused by stimulation of interleukin-1.beta. production, such as immune system diseases, inflammatory diseases, and ischemic diseases.

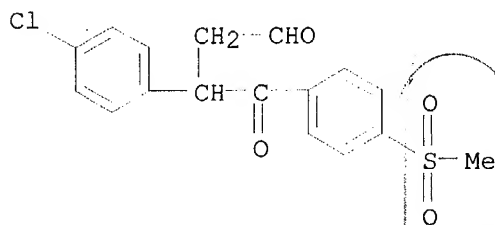
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 388606-95-9P

(prepn. of phenylpyridazine derivs. as inhibitors of interleukin 1.beta. prodn. and preventive and therapeutic drugs for diseases caused by increased prodn. of interleukin 1.beta.)

RN 388606-95-9 USPATFULL

CN Benzenebutanal, .beta.-(4-chlorophenyl)-4-(methylsulfonyl)-.gamma.-oxo-  
 (9CI) (CA INDEX NAME)



L11 ANSWER 21 OF 31 USPATFULL on STN

ACCESSION NUMBER: 2002:338219 USPATFULL

TITLE: Azepine derivatives having effects on serotonin related systems

INVENTOR(S): Hauser, Kenneth Lee, Greencastle, IN, UNITED STATES  
 Hertel, Larry Wayne, Indianapolis, IN, UNITED STATES  
 Xu, Yao-Chang, Fishers, IN, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002193590	A1	20021219
APPLICATION INFO.:	US 2002-141424	A1	20020508 (10)
RELATED APPLN. INFO.:	Division of Ser. No. US 2000-701363, filed on 28 Nov 2000, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-91245P	19980630 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ELI LILLY AND COMPANY, PATENT DIVISION, P.O. BOX 6288, INDIANAPOLIS, IN, 46206-6288	
NUMBER OF CLAIMS:	23	
EXEMPLARY CLAIM:	1	
LINE COUNT:	2981	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides compounds of formula I and a method of inhibiting the reuptake of serotonin, antagonizing the 5-HT.sub.1A

receptor and antagonizing the 5-HT.sub.2A receptor which comprises administering to a subject in need of such treatment an effective amount of a compound of formula I.

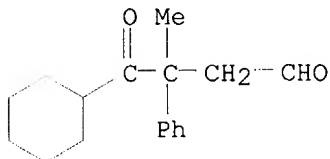
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 228419-04-3P

(prepn. of azepine derivs. having effects on serotonin related systems)

RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 22 OF 31 USPATFULL on STN

ACCESSION NUMBER: 2002:301625 USPATFULL

TITLE: Arylpiperazines having activity at the serotonin 1A receptor

INVENTOR(S): Godfrey, Alexander Glenn, Greenwood, IN, UNITED STATES  
Kohlman, Daniel Timothy, Indianapolis, IN, UNITED STATES

O' Toole, John Cunningham, Indianapolis, IN, UNITED STATES

Xu, Yao-Chang, Fishers, IN, UNITED STATES

Zhang, Tony Yantao, Indianapolis, IN, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002169170	A1	20021114
	US 6645967	B2	20031111
APPLICATION INFO.:	US 2001-22045	A1	20011218 (10)
RELATED APPLN. INFO.:	Division of Ser. No. US 2001-753645, filed on 3 Jan 2001, GRANTED, Pat. No. US 6358958		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-89589P	19980617 (60)
	US 1997-69722P	19971216 (60)
	US 1997-69791P	19971216 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ELI LILLY AND COMPANY, PATENT DIVISION, P.O. BOX 6288, INDIANAPOLIS, IN, 46206-6288	
NUMBER OF CLAIMS:	4	
EXEMPLARY CLAIM:	55	
LINE COUNT:	1970	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A method for potentiating the action of a serotonin reuptake inhibitor in increasing the availability of serotonin, norepinephrin and dopamine in the brain, comprising administering to a patient in need of such treatment a serotonin reuptake inhibitor in combination with an effective amount of a compound of the formula ##STR1##

wherein

Ar' is a mono or bicyclic aryl or heteroaryl radical substituted with

one to three substituents selected from the group consisting of hydrogen, (C.sub.1-C.sub.6)alkyl, (C.sub.1-C.sub.6)alkoxy, (C.sub.1-C.sub.6)alkylthio, (C.sub.2-C.sub.6)alkenyl, (C.sub.2-C.sub.6)alkynyl, (C.sub.1-C.sub.6)alkyl halo, (C.sub.3-C.sub.8)cycloalkyl, (C.sub.3-C.sub.8)cycloalkenyl or halo;

R.sub.1 is hydrogen, (C.sub.1-C.sub.6)alkyl, (C.sub.1-C.sub.6)alkoxy, (C.sub.1-C.sub.6)alkylthio;

R.sub.2 is phenyl, naphthyl or (C.sub.3-C.sub.12)cycloalkyl substituted with one or two substituents selected from the group consisting of hydrogen (C.sub.1-C.sub.6)alkyl, (C.sub.1-C.sub.6)alkoxy, (C.sub.1-C.sub.6)alkylthio, (C.sub.2-C.sub.6)alkenyl, (C.sub.2-C.sub.6)alkynyl, (C.sub.1-C.sub.6)alkyl halo, (C.sub.3-C.sub.8)cycloalkyl, (C.sub.3-C.sub.8)cycloalkenyl or halo;

R.sub.3 is selected from the group consisting of hydrogen (C.sub.1-C.sub.6)alkyl, (C.sub.1-C.sub.6)alkoxy, (C.sub.1-C.sub.6)alkylthio, (C.sub.2-C.sub.6)alkenyl, (C.sub.2-C.sub.6)alkynyl, (C.sub.1-C.sub.6)alkyl halo, (C.sub.3-C.sub.8)cycloalkyl, (C.sub.3-C.sub.8)cycloalkenyl or halo;

X is --(C.dbd.O)--, --CHOH-- or --CH.sub.2--;

or a pharmaceutically acceptable salt, racemate, optical isomer or solvate thereof.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

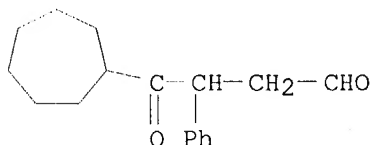
IT 228419-09-8, 3-Cycloheptanecarbonyl-3-phenylpropanal

228419-10-1, 3-Cyclopentanecarbonyl-3-phenylpropanal

(prepn. of arylpiperazines having activity at serotonin 1a receptor)

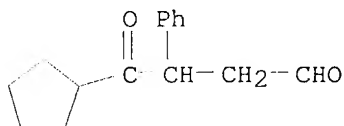
RN 228419-09-8 USPATFULL

CN Cycloheptanebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-10-1 USPATFULL

CN Benzenepropanal, .beta.-(cyclopentylcarbonyl)- (9CI) (CA INDEX NAME)



IT 147031-23-0P, 3-Benzoyl-3-phenylpropionaldehyde

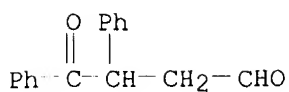
228418-97-1P, 3-Cyclohexanecarbonyl-3-propanal

228419-00-9P, 3-Benzoyl-3-phenylbutanal 228419-04-3P

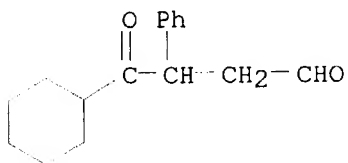
(prepn. of arylpiperazines having activity at serotonin 1a receptor)

RN 147031-23-0 USPATFULL

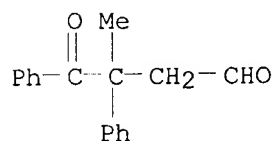
CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



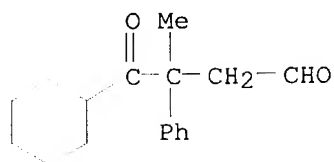
RN 228418-97-1 USPATFULL  
 CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)- (9CI) (CA INDEX NAME)



RN 228419-00-9 USPATFULL  
 CN Benzenebutanal, .beta.-methyl-.gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-04-3 USPATFULL  
 CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 23 OF 31 USPATFULL on STN  
 ACCESSION NUMBER: 2002:268750 USPATFULL  
 TITLE: Azepine derivatives having effects on serotonin related systems  
 INVENTOR(S): Hauser, Kenneth Lee, Greencastle, IN, United States  
 Hertel, Larry Wayne, Indianapolis, IN, United States  
 Xu, Yao-Chang, Fishers, IN, United States  
 PATENT ASSIGNEE(S): Eli Lilly and Company, Indianapolis, IN, United States  
 (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6465453	B1	20021015
	WO 2000000203		20000106
APPLICATION INFO.:	US 2000-701363		20001128 (9)
	WO 1999-US14778		19990629
			19990629 PCT 371 date

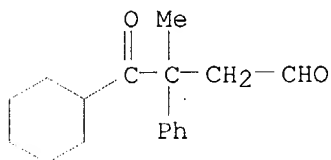
	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-91245P	19980630 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Coleman, Brenda	
LEGAL REPRESENTATIVE:	Joyner, Charles T., Lentz, Nelsen L.	
NUMBER OF CLAIMS:	19	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)	
LINE COUNT:	2882	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides compounds of formula I and a method of inhibiting the reuptake of serotonin, antagonizing the 5-HT.sub.1A receptor and antagonizing the 5-HT.sub.2A receptor which comprises administering to a subject in need of such treatment an effective amount of a compound of formula I.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 228419-04-3P  
 (prepn. of azepine derivs. having effects on serotonin related systems)  
 RN 228419-04-3 USPATFULL  
 CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 24 OF 31 USPATFULL on STN  
 ACCESSION NUMBER: 2002:209547 USPATFULL  
 TITLE: Piperidine derivatives having effects on serotonin related systems  
 INVENTOR(S): Hertel, Larry Wayne, Indianapolis, IN, United States  
 Kohlman, Daniel Timothy, Camby, IN, United States  
 Liang, Sidney Xi, Fishers, IN, United States  
 Wong, David Taiwai, Indianapolis, IN, United States  
 Xu, Yao-Chang, Fishers, IN, United States  
 PATENT ASSIGNEE(S): Eli Lilly and Company, Indianapolis, IN, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6436964	B1	20020820
	WO 2000000198		20000106
APPLICATION INFO.:	US 2000-701406		20001128 (9)
	WO 1999-US14732		19990629
			20001128 PCT 371 date

	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-91241P	19980630 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Fan, Jane	
LEGAL REPRESENTATIVE:	Joyner, Charles T., Lentz, Nelsen L.	
NUMBER OF CLAIMS:	25	

EXEMPLARY CLAIM: 1  
 NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)  
 LINE COUNT: 3433  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
 AB The present invention provides the compounds of the following formula:

Wherein the variables are as defined in the specification and a method for inhibiting the reuptake of serotonin, antagonizing the 5-HT.sub.1A receptor and antagonizing the 5-HT.sub.2A receptor which comprises administering to a subject in need of such treatment an effective amount of the compound of above formula.

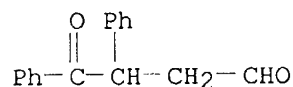
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 147031-23-0P 228419-04-3P

(prepn. of piperidine derivs. having effects on serotonin related systems)

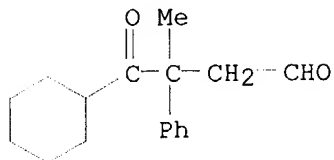
RN 147031-23-0 USPATFULL

CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 25 OF 31 USPATFULL on STN

ACCESSION NUMBER: 2002:45628 USPATFULL

TITLE: Pyrrolidine and pyrroline derivatives having effects on serotonin related systems

INVENTOR(S): Hertel, Larry Wayne, Indianapolis, IN, United States  
 Xu, Yao-Chang, Fishers, IN, United States

PATENT ASSIGNEE(S): Eli Lilly and Company, Indianapolis, IN, United States  
 (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6353008	B1	20020305
	WO 2000000196		20000106
APPLICATION INFO.:	US 2000-701361		20001128 (9)
	WO 1999-US14881		19990629
			20001128 PCT 371 date

	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-91204P	19980630 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Fan, Jane	
LEGAL REPRESENTATIVE:	Joyner, Charles T., Lentz, Nelson L.	

NUMBER OF CLAIMS: 17  
 EXEMPLARY CLAIM: 1  
 NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)  
 LINE COUNT: 2949

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides the compounds of the following formula  
 (I): ##STR1##

and a method for inhibiting the reuptake of serotonin, antagonizing the 5-HT.sub.1A receptor and antagonizing the 5-HT.sub.2A receptor which comprises administering to a subject in need of such treatment an effective amount of formula (I).

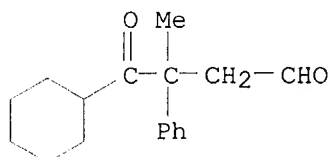
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 228419-04-3P

(prepn. of pyrrolidine and pyrroline derivs. having effects on serotonin related systems)

RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 26 OF 31 USPATFULL on STN

ACCESSION NUMBER: 2001:91599 USPATFULL

TITLE: Arylpiperazines having activity at the serotonin 1A receptor

INVENTOR(S): Godfrey, Alexander Glenn, Greenwood, IN, United States  
 Kohlman, Daniel Timothy, Indianapolis, IN, United States  
 O'Toole, John Cunningham, Indianapolis, IN, United States  
 Xu, Yao-Chang, Fishers, IN, United States  
 Zhang, Tony Yantao, Indianapolis, IN, United States

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2001003749	A1	20010614
	US 6358958	B2	20020319
APPLICATION INFO.:	US 2001-753645	A1	20010103 (9)
RELATED APPLN. INFO.:	Division of Ser. No. US 1998-208553, filed on 9 Dec 1998, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1998-89589P	19980617 (60)
	US 1997-69722P	19971216 (60)
	US 1997-69791P	19971216 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	NELSEN L. LENTZ, Eli Lilly and Company, Lilly Corporate Center, Patent Division DC: 1104, Indianapolis, IN, 46285	
NUMBER OF CLAIMS:	45	
EXEMPLARY CLAIM:	1	



LINE COUNT: 2215

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A series of aryl piperazine compounds are effective pharmaceuticals for the treatment of conditions related to or affected by the serotonin 1.sub.A receptor; the compounds are particularly effective antagonists at that receptor, and are particularly useful for alleviating the symptoms of nicotine and tobacco withdrawal.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

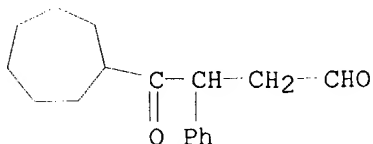
IT 228419-09-8, 3-Cycloheptanecarbonyl-3-phenylpropanal

228419-10-1, 3-Cyclopentanecarbonyl-3-phenylpropanal

(prepn. of arylpiperazines having activity at serotonin 1a receptor)

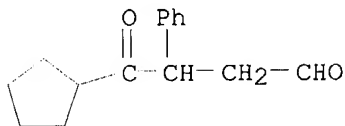
RN 228419-09-8 USPATFULL

CN Cycloheptanebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-10-1 USPATFULL

CN Benzenepropanal, .beta.-(cyclopentylcarbonyl)- (9CI) (CA INDEX NAME)



IT 147031-23-0P, 3-Benzoyl-3-phenylpropionaldehyde

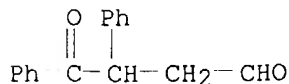
228418-97-1P, 3-Cyclohexanecarbonyl-3-propanal

228419-00-9P, 3-Benzoyl-3-phenylbutanal 228419-04-3P

(prepn. of arylpiperazines having activity at serotonin 1a receptor)

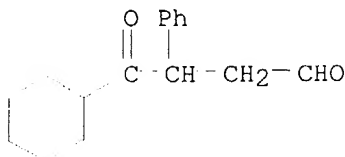
RN 147031-23-0 USPATFULL

CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



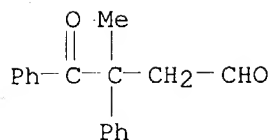
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CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)- (9CI) (CA INDEX NAME)

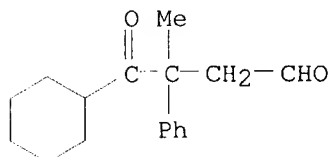


RN 228419-00-9 USPATFULL

CN Benzenebutanal, .beta.-methyl-.gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-04-3 USPATFULL  
CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA  
INDEX NAME)



L11 ANSWER 27 OF 31 USPATFULL on STN  
ACCESSION NUMBER: 2001:79160 USPATFULL  
TITLE: Arylpiperazines having activity at the serotonin 1A  
receptor  
INVENTOR(S): Kohlman, Daniel Timothy, Indianapolis, IN, United  
States  
Xu, Yao-Chang, Fishers, IN, United States  
PATENT ASSIGNEE(S): Eli Lilly and Company, Indianapolis, IN, United States  
(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6239135	B1	20010529
APPLICATION INFO.:	US 1998-208553		19981209 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 1997-69722P	19971216 (60)
	US 1997-69791P	19971216 (60)
	US 1998-89589P	19980617 (60)

DOCUMENT TYPE: Utility  
FILE SEGMENT: Granted  
PRIMARY EXAMINER: Bernhart, Emily  
LEGAL REPRESENTATIVE: Lentz, Nelsen L., Palmberg, Arleen  
NUMBER OF CLAIMS: 8  
EXEMPLARY CLAIM: 1  
LINE COUNT: 1894

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

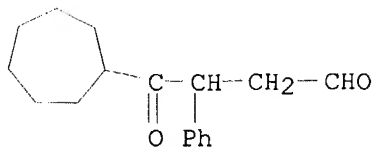
AB A series of aryl piperazine compounds of the formula: ##STR1##

or the pharmaceutically acceptable salts thereof, are effective  
pharmaceuticals for the treatment of conditions related to or affected  
by the serotonin 1.sub.A receptor; the compounds are particularly  
effective antagonists at that receptor, and are particularly useful for  
alleviating the symptoms of nicotine and tobacco withdrawal.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

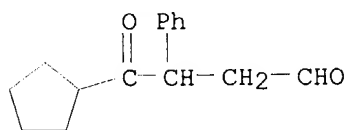
IT 228419-09-8, 3-Cycloheptanecarbonyl-3-phenylpropanal  
228419-10-1, 3-Cyclopentanecarbonyl-3-phenylpropanal  
(prepn. of arylpiperazines having activity at serotonin 1a receptor)  
RN 228419-09-8 USPATFULL

CN Cycloheptanebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-10-1 USPATFULL

CN Benzenepropanal, .beta.-(cyclopentylcarbonyl)- (9CI) (CA INDEX NAME)



IT 147031-23-0P, 3-Benzoyl-3-phenylpropionaldehyde

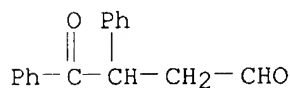
228418-97-1P, 3-Cyclohexanecarbonyl-3-propanal

228419-00-9P, 3-Benzoyl-3-phenylbutanal 228419-04-3P

(prepn. of arylpiperazines having activity at serotonin 1a receptor)

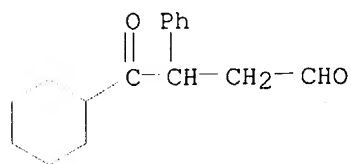
RN 147031-23-0 USPATFULL

CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



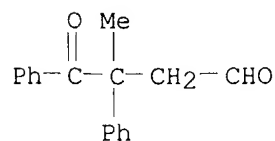
RN 228418-97-1 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)- (9CI) (CA INDEX NAME)



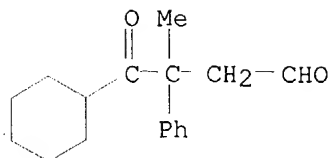
RN 228419-00-9 USPATFULL

CN Benzenebutanal, .beta.-methyl-.gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 28 OF 31 USPATFULL on STN  
 ACCESSION NUMBER: 2000:49626 USPATFULL  
 TITLE: Line marking shoe  
 INVENTOR(S): McGuffie, Iain Peter, Hungry Hill Farm, Stoke Lacy, NR  
 Bromyard, Herefordshire HR7 4HD, United Kingdom

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6053376		20000425
	WO 9721871		19970619
APPLICATION INFO.:	US 1998-91204		19980610 (9)
	WO 1996-GB2323		19960920
			19980610 PCT 371 date
			19980610 PCT 102(e) date

	NUMBER	DATE
PRIORITY INFORMATION:	GB 1995-25431	19951213
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Shaver, Kevin	
ASSISTANT EXAMINER:	Bui, Thach	
LEGAL REPRESENTATIVE:	Dorman, Ira S.	
NUMBER OF CLAIMS:	23	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	4 Drawing Figure(s); 2 Drawing Page(s)	
LINE COUNT:	451	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A line marking shoe (1) adapted in use to be advanced relative to a ground surface in a line marking direction to mark a line onto the ground surface in the line marking direction (A) includes a sole part (3) having a discharge opening region (13) formed in it for discharge of line marking material onto the ground surface. The discharge opening region includes a number of discharge opening areas and the discharge opening areas are so dimensioned and arranged that discharge of line marking material onto the ground surface through different discharge opening areas produces lines of different widths on the ground surface.

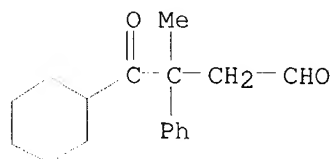
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 228419-04-3P

(prepn. of pyrrolidine and pyrroline derivs. having effects on serotonin related systems)

RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 29 OF 31 USPATFULL on STN  
 ACCESSION NUMBER: 2000:45719 USPATFULL  
 TITLE: Method for forming a packaging for a plurality of  
 containers which is easily opened  
 INVENTOR(S): Loreto, Vittorino, Siracusa, Italy  
 Loreto, Corrado, Avola, Italy  
 PATENT ASSIGNEE(S): Cielle Di Loreto Tommaso, Mililli, Italy (non-U.S.  
 corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6050058		20000418
	WO 9721608		19970619
APPLICATION INFO.:	US 1998-91241		19980612 (9)
	WO 1996-EP5545		19961211
			19980612 PCT 371 date
			19980612 PCT 102(e) date

	NUMBER	DATE
PRIORITY INFORMATION:	IT 1995-MI2595	19951212
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Vo, Peter	
ASSISTANT EXAMINER:	Luby, Matthew	
LEGAL REPRESENTATIVE:	Young & Thompson	
NUMBER OF CLAIMS:	6	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	4 Drawing Figure(s); 2 Drawing Page(s)	
LINE COUNT:	303	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The method for forming a packaging (1) for a plurality of containers (2) arranged in lines and rows involves wrapping the group of containers with a section of heat-sealable plastic film (3), the two end flaps of which overlap so as to be able to be heat-sealed with one another. Pre-cut lines (5), parallel to the direction in which the film itself extends, are formed beforehand in the film. The pre-cut lines are positioned at a distance from one another and, in the finished packaging, each pre-cut line is arranged between two adjacent rows of containers. One side of the film used is provided, in the position where a longitudinal pre-cut lines is already present or is to be formed, with a strip-shaped area which is not heat-sealable when it comes into contact with the film itself. The width of the strips which are not heat-sealable is chosen so as to cover the maximum overlapping imprecision due to the packaging machines.

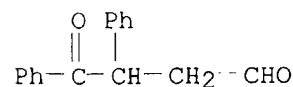
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 147031-23-0P 228419-04-3P

(prepn. of piperidine derivs. having effects on serotonin related systems)

RN 147031-23-0 USPATFULL

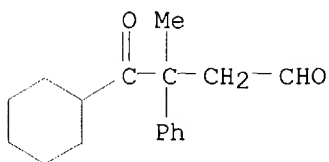
CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA

INDEX NAME)



L11 ANSWER 30 OF 31 USPATFULL on STN  
ACCESSION NUMBER: 2000:32951 USPATFULL  
TITLE: Men's body temperature controlling pants  
INVENTOR(S): Chung, Seun Yung, Kocheung Jukong Apt. 1313-203, Haan  
3-Dong, Kwangmyung City, Kyungki-do, 423-060, Korea,  
Republic of

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6038703		20000321
	WO 9721363		19970619
APPLICATION INFO.:	US 1998-91245		19980612 (9)
	WO 1996-KR238		19961211
			19980612 PCT 371 date
			19980612 PCT 102(e) date

	NUMBER	DATE
PRIORITY INFORMATION:	KR 1995-U41021	19951212
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Hale, Gloria M.	
LEGAL REPRESENTATIVE:	Wenderoth, Lind & Ponack, L.L.P.	
NUMBER OF CLAIMS:	12	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	5 Drawing Figure(s); 2 Drawing Page(s)	
LINE COUNT:	148	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Men's pants (shorts or briefs) have a Y type separation band (2) or a U type separation band (22) inside thereof together with separation pads (7, 77) to separate the testicles from the body, the penis from the testicles, and the penis from both hips. Complete separation around the male genitals is achieved without effort by wearing these pants. A penis band (3) formed with an elastic band (4, 44) and clips (5, 55) is sewn to a center part of a waist band (6) in an I shape. A penis hole (14) can be adjusted by moving the two clips (5, 55) up and down according to the individual location and size of the penis (101). A lower part (88) below the clip (5) helps to increase separation between the testicles and the penis.

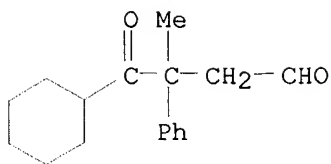
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 228419-04-3P

(prepn. of azepine derivs. having effects on serotonin related systems)

RN 228419-04-3 USPATFULL

CN Benzenepropanal, .beta.-(cyclohexylcarbonyl)-.beta.-methyl- (9CI) (CA  
INDEX NAME)



L11 ANSWER 31 OF 31 USPATFULL on STN  
 ACCESSION NUMBER: 94:20167 USPATFULL  
 TITLE: Pyrrolopyrazine derivatives  
 INVENTOR(S): Rover, Stephan, Grenzach-Wyhlen, Germany, Federal Republic of  
 PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., Nutley, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5292732		19940308
APPLICATION INFO.:	US 1992-905584		19920626 (7)

	NUMBER	DATE
PRIORITY INFORMATION:	CH 1991-1950	19910702
	CH 1992-1667	19920522

DOCUMENT TYPE: Utility  
 FILE SEGMENT: Granted  
 PRIMARY EXAMINER: Berch, Mark L.  
 LEGAL REPRESENTATIVE: Gould, George M., Johnston, George W., Parise, John P.  
 NUMBER OF CLAIMS: 13  
 EXEMPLARY CLAIM: 1,12,13  
 LINE COUNT: 2905

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The novel pyrrolopyrazines of the general formula ##STR1## wherein one of R.sup.1 and R.sup.2 signifies aryl and the other signifies hydrogen, lower alkyl or aryl or R.sup.1 and R.sup.2 together with the two carbon atoms denoted by .alpha. and .beta. signify the group A; ##STR2## R.sup.3 signifies hydrogen or lower alkyl and R.sup.4 signifies hydrogen or

R.sup.3 and R.sup.4 together signify an additional C/N bond;

R.sup.5 signifies hydrogen or lower alkyl;

R.sup.6 signifies hydrogen or lower alkyl;

R.sup.7 signifies hydrogen, halogen, lower alkyl, optionally substituted lower alkoxy, or C.sub.3-6 -cycloalkyl, C.sub.4-6 -cycloalkenyl, C.sub.3-6 -cycloalkyloxy, hydroxy, trifluoro- methanesulphonyloxy or optionally substituted benzyl- oxycarbonyloxy; and the dotted line signifies an optional additional C/C bond,

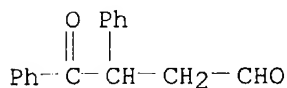
and pharmaceutically acceptable acid addition salts of the compounds of formula I can be used in the control or prevention of illnesses or in the improvement of health, especially in the control or prevention of depressive states, cognitive disorders and neurodegenerative diseases such as Parkinson's disease and Alzheimer's disease.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 147031-23-0P

(prepn. of, as intermediate for pyrrolopyrazine deriv. monoamine

oxidase inhibitor)  
RN 147031-23-0 USPATFULL  
CN Benzenebutanal, .gamma.-oxo-.beta.-phenyl- (9CI) (CA INDEX NAME)



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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

L3 STR  
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L10 0 SEA FILE=CAOLD ABB=ON L7



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 FILE 'CASREACT' ENTERED AT 16:30:03 ON 27 FEB 2004  
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FILE CONTENT:1840 - 22 Feb 2004 VOL 140 ISS 8

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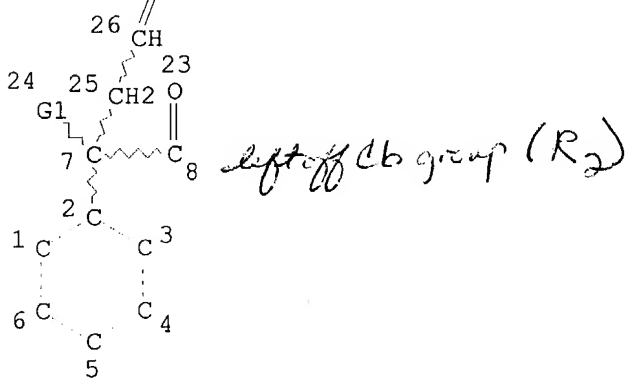
This file contains CAS Registry Numbers for easy and accurate substance identification.

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Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

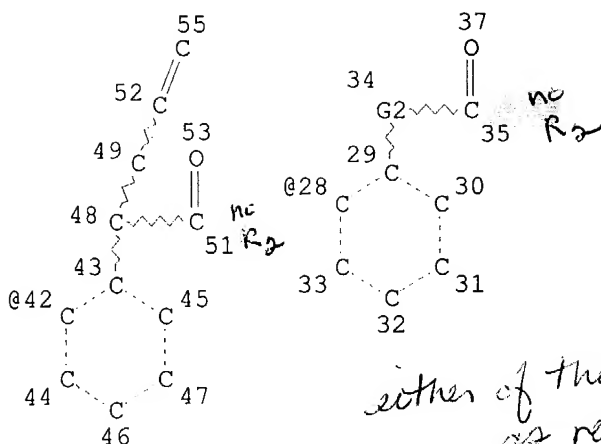
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CH~Ak CH~O~Ak CH~S~Ak  
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Page 1-A



Page 2-A

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VAR G2=CH2/57/59/62

VAR G3=42/28

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

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6 DOCS

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L20 ANSWER 1 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 140:28052 CASREACT

TITLE: Asymmetric synthesis of aminopyrrolidinones

INVENTOR(S): Waltermire, Robert E.; Savage, Scott A.; Campagna, Silvio; Magnus, Nicholas A.; Confalone, Pasquale N.; Yates, Matthew; Meloni, David J.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 65 pp.

CODEN: PIXXD2

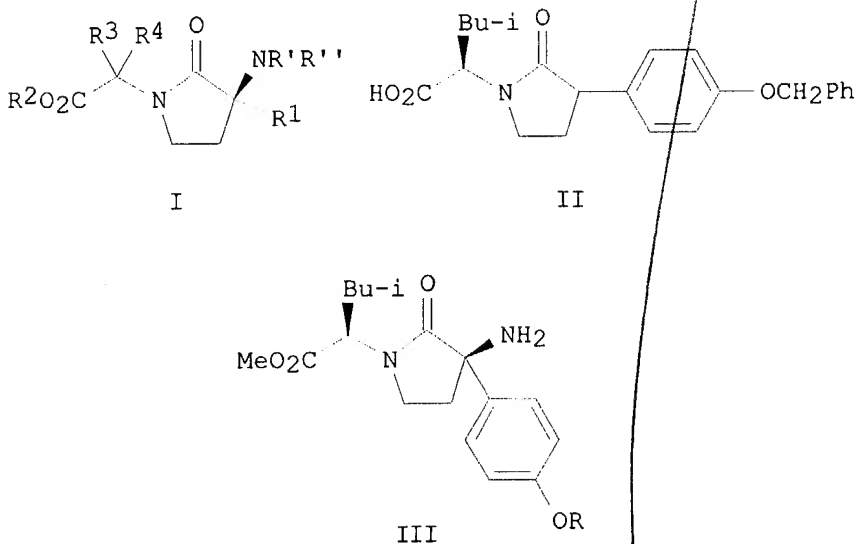
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LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

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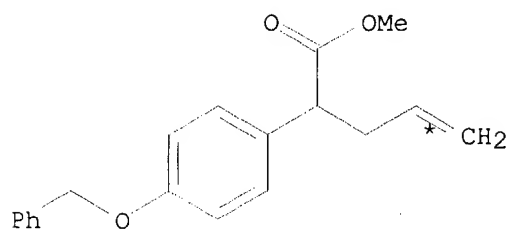
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US 2003236401	A1	20031225	US 2003-389528	20030314
PRIORITY APPLN. INFO.:			US 2002-387637P	20020611
OTHER SOURCE(S):			MARPAT 140:28052	
GI				



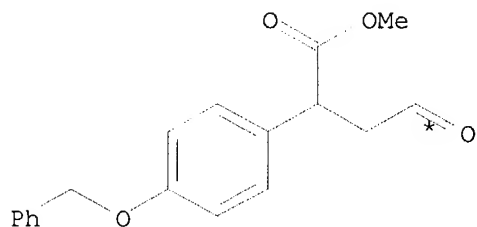
AB A novel process for the asym. synthesis of an aminopyrrolidinones I [R' is H, (cyclo)alkyl; R'' is a group R' or OH; R<sub>1</sub> is substituted Ph or pyridyl; R<sub>2</sub> is H, alkyl, Ph, benzyl; R<sub>3</sub> is H, Q, (oxa)(aza)alk(en)(yn)ylene-Q, where Q is (un)substituted carbocyclyl; R<sub>4</sub> is (oxa)(aza)alk(en)(yn)ylene-H] and corresponding aminoazetidinone, aminopiperidinone, and aminohexahydroazepinone analogs involves amination of corresponding pyrrolidinones or analogs. The products are useful as intermediates for MMP and TACE inhibitors. Thus, pyrrolidinone II was prepd. by cyclocondensation of p-PhCH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CH(CH<sub>2</sub>CHO)CO<sub>2</sub>Me with D-leucine Me ester hydrochloride. Amination of II with 1-chloro-1-nitrosocyclopentane, followed by catalytic hydrogenation in MeOH, mesylation, N-protection with p-tolualdehyde, and reaction with 4-(chloromethyl)-2-methylquinoline (R-Cl) afforded III (isolated as the HCl salt).

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 47 ...A ==&gt; B...



A

(1)  $\xrightarrow{\hspace{1cm}}$ 

B

YIELD 80%

RX(1) RCT A 223410-63-7

STAGE(1)

RGT C 10028-15-6 Ozone

SOL 141-78-6 AcOEt

STAGE(2)

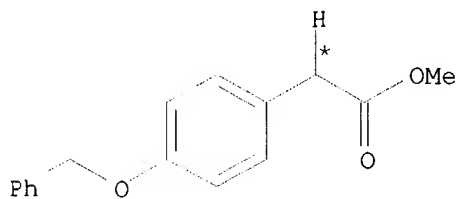
RGT D 64-19-7 AcOH, E 7440-66-6 Zn

SOL 7732-18-5 Water

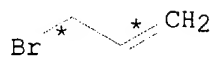
PRO B 634196-85-3

RX(17) OF 47 COMPOSED OF RX(6), RX(1)

RX(17) AH + AI ==&gt; B

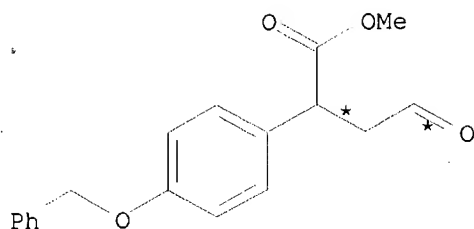


AH



AI

2  
STEPS  
 $\xrightarrow{\hspace{1cm}}$



B  
YIELD 80%

RX(6) RCT AH 68641-16-7

STAGE(1)

RGT AJ 4111-54-0 LiN(Pr-i)<sub>2</sub>

SOL 109-99-9 THF

STAGE(2)

RCT AI 106-95-6

PRO A 223410-63-7

RX(1) RCT A 223410-63-7

STAGE(1)

RGT C 10028-15-6 Ozone

SOL 141-78-6 AcOEt

STAGE(2)

RGT D 64-19-7 AcOH, E 7440-66-6 Zn

SOL 7732-18-5 Water

PRO B 634196-85-3

=> d ibib abs hit 2-6; fil hom

L20 ANSWER 2 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 138:55826 CASREACT

TITLE: Discovery of .gamma.-Lactam Hydroxamic Acids as  
Selective Inhibitors of Tumor Necrosis Factor .alpha.  
Converting Enzyme: Design, Synthesis, and  
Structure-Activity Relationships

AUTHOR(S): Duan, James J. W.; Chen, Lihua; Wasserman, Zelda R.;  
Lu, Zhonghui; Liu, Rui-Qin; Covington, Maryanne B.;  
Qian, Mingxin; Hardman, Karl D.; Magolda, Ronald L.;  
Newton, Robert C.; Christ, David D.; Wexler, Ruth R.;  
Decicco, Carl P.

CORPORATE SOURCE: Discovery Chemistry, Experimental Station,  
Bristol-Myers Squibb Company, Wilmington, DE,  
19880-0500, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(23),  
4954-4957

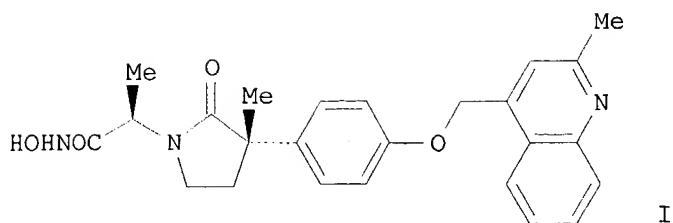
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

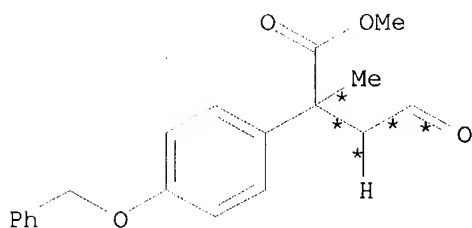
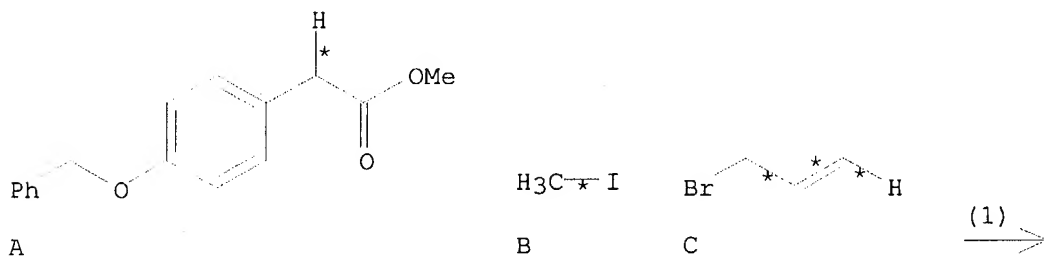
GI



AB New .gamma.-lactam TACE inhibitors were designed from known MMP inhibitors. A homol. model of TACE was built and examd. to identify the S1' site as the key area for TACE selectivity over MMPs. Rational exploration of the P1'-S1' interactions resulted in the discovery of the 3,5-disubstituted benzyl ether as a TACE-selective P1' group. Further optimization led to the discovery of IK682 (I) as a selective and orally bioavailable TACE inhibitor.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 10 A + B + C ==> D...



D  
YIELD 82%

RX(1) RCT A 68641-16-7

STAGE(1)

RGT E 1070-89-9 (Me3Si)2N.Na

SOL 109-99-9 THF

STAGE(2)

RCT B 74-88-4

STAGE(3)

RGT F 12125-02-9 NH4Cl  
SOL 7732-18-5 Water

STAGE(4)  
RGT E 1070-89-9 (Me3Si)2N.Na  
SOL 109-99-9 THF

STAGE(5)  
RCT C 106-95-6

STAGE(6)  
RGT F 12125-02-9 NH4Cl  
SOL 7732-18-5 Water

STAGE(7)  
RGT G 10028-15-6 Ozone

STAGE(8)  
RGT H 603-35-0 PPh3  
PRO D 223406-00-6

L20 ANSWER 3 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 134:366781 CASREACT

TITLE: Diastereoselective synthesis of substituted  
tetrahydroquinoline-4-carboxylic esters by a tandem  
reduction-reductive amination reaction

AUTHOR(S): Bunce, Richard A.; Herron, Derrick M.; Johnson, Lara  
B.; Kotturi, Sharadsrikar V.

CORPORATE SOURCE: Department of Chemistry, Oklahoma State University,  
Stillwater, OK, 74078-3071, USA

SOURCE: Journal of Organic Chemistry (2001), 66(8), 2822-2827  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

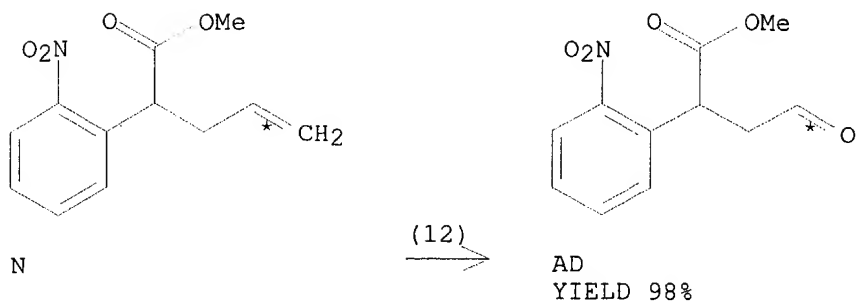
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A diastereoselective synthesis of cis-1-methyl-2-alkyl-1,2,3,4-  
tetrahydroquinoline-4-carboxylic acids and cis-2-alkyl-1,2,3,4-  
tetrahydroquinoline-4-carboxylic esters was developed from Me  
(2-nitrophenyl)acetate (I). The method involves alkylation of I with an  
allylic halide, ozonolysis of the double bond, and catalytic  
hydrogenation. The final hydrogenation initiates a tandem sequence  
involving redn. of the arom. nitro group, condensation of the aniline or  
hydroxylamine nitrogen with the side chain carbonyl group, redn. of the  
resulting nitrogen intermediate, and reductive amination of the  
tetrahydroquinoline with formaldehyde produced in the ozonolysis to give a  
Me (.+-.)-1-methyl-2-alkyl-1,2,3,4-tetrahydroquinoline-4-carboxylate.  
Removal of the formaldehyde prior to hydrogenation gives the simple  
(.+-.)-2-alkyl derivs. The products were isolated in high yield as single  
diastereomers having the C-2 alkyl group cis to the C-4 carboxylic ester.  
The reaction was extended to the synthesis of tricyclic structures with  
similar high diastereoselection.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(12) OF 50 ...N ==> AD...



RX(12) RCT N 274676-13-0

STAGE(1)

RGT T 10028-15-6 Ozone

SOL 67-56-1 MeOH

STAGE(2)

RGT AE 75-18-3 Me2S

STAGE(3)

RGT AF 104-15-4 TsOH

STAGE(4)

SOL 60-29-7 Et2O

STAGE(5)

RGT AG 7601-90-3 HClO4

SOL 109-99-9 THF

STAGE(6)

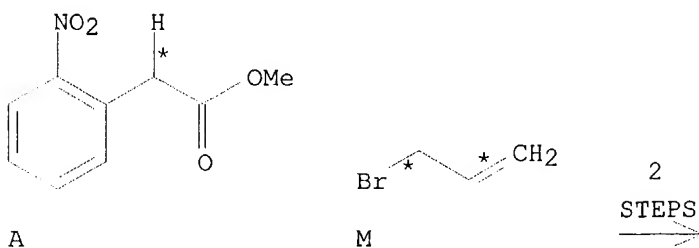
SOL 75-09-2 CH2Cl2

PRO AD 340269-83-2

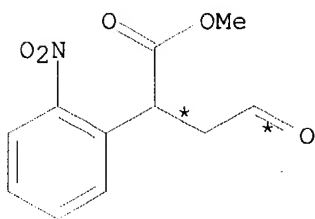
NTE stereoselective

RX(34) OF 50 COMPOSED OF RX(5), RX(12)

RX(34) A + M ==> AD







AD  
YIELD 98%

RX(5) RCT A 30095-98-8

STAGE(1)

RGT D 584-08-7 K2CO3  
CAT 17455-13-9 18-Crown-6  
SOL 75-05-8 MeCN

STAGE(2)

RCT M 106-95-6  
SOL 75-05-8 MeCN  
PRO N 274676-13-0  
NTE stereoselective

RX(12) RCT N 274676-13-0

STAGE(1)

RGT T 10028-15-6 Ozone  
SOL 67-56-1 MeOH

STAGE(2)

RGT AE 75-18-3 Me2S

STAGE(3)

RGT AF 104-15-4 TsOH

STAGE(4)

SOL 60-29-7 Et2O

STAGE(5)

RGT AG 7601-90-3 HClO4  
SOL 109-99-9 THF

STAGE(6)

SOL 75-09-2 CH2Cl2  
PRO AD 340269-83-2  
NTE stereoselective

L20 ANSWER 4 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

116:255827 CASREACT

TITLE:

Asymmetric construction of quaternary carbons from chiral malonates: selective and versatile total syntheses of the enantiomers of .alpha.- and .beta.-cuparenes from a common optically active precursor.

AUTHOR(S):

Canet, Jean Louis; Fadel, Antoine; Salaun, Jacques

CORPORATE SOURCE:

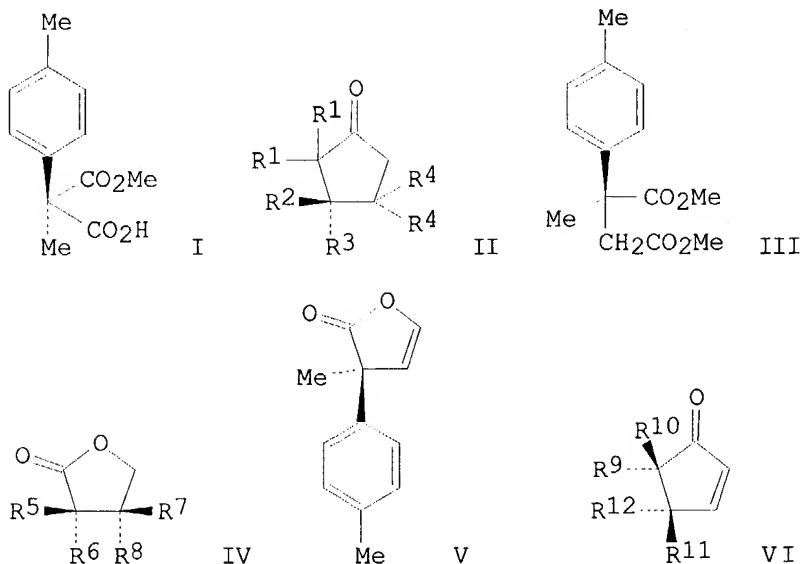
Inst. Chim. Mol., Univ. Paris-Sud, Orsay, 91405, Fr.

SOURCE:

Journal of Organic Chemistry (1992), 57(12), 3463-73

DOCUMENT TYPE:  
LANGUAGE:  
GI

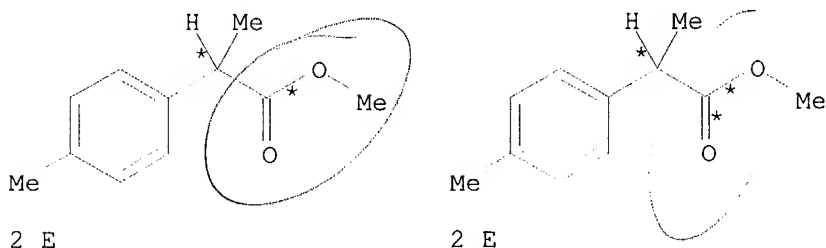
CODEN: JOCEAH; ISSN: 0022-3263  
Journal  
English

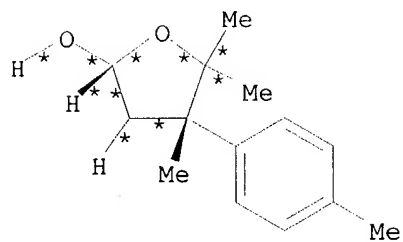
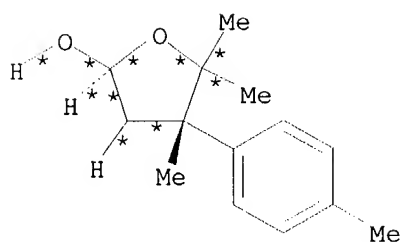
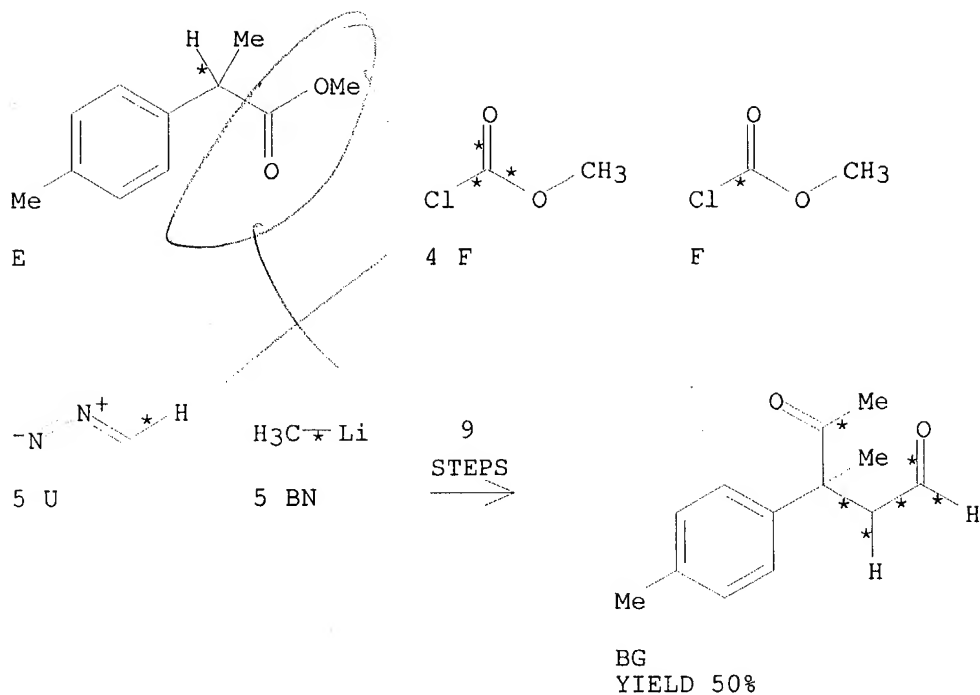


AB From single chiron (R)-I, available with high enantiomeric purity (96%) by simple enzymic hydrolysis (PLE) of a prochiral malonate, were prepd. convenient precursors of the two enantiomers of .alpha.- (II; R1 = R3 = Me, R2 = p-MeC6H4, R4 = H; R1 = R2 = Me, R3 = p-MeC6H4, R4 = H) and .beta.-cuparenes (II; R1 = H, R2 = p-MeC6H4, R3 = R4 = Me; R1 = H, R2 = R4 = Me, R3 = p-MeC6H4). This versatile method also allows preps. of the enantiomer (S)-I and di-Me 2-methyl-2-p-tolylsuccinate [(S)-III] as well as the new butyrolactones (R)-IV (R5 = p-MeC6H4, R6 = Me, R7R8 = O; R5 = R6 = H, R7 = p-MeC6H4, R8 = Me) and (S)-IV (R5 = p-MeC6H4, R6 = Me, R7 = R8 = H), the new but-3-enolide (S)-V, and cyclopentenones (S)-VI (R9 = R10 = H, R11 = p-MeC6H4, R12 = Me; R9 = p-MeC6H4, R10 = Me, R11 = R12 = H), all bearing an asym. quaternary carbon.

RX(439) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(7), RX(22), RX(30), RX(23), RX(24)

RX(439) 5 E + 5 F + 5 U + 5 BN ==> BG + BO + BP





RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi  
SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1  
PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
 RGT L 1310-73-2 NaOH  
 PRO K 127047-05-6  
 CAT 9013-79-0 Esterase  
 SOL 7732-18-5 Water  
 NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
 RGT AM 79-37-8 (COCl)<sub>2</sub>

PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et2O

RX(7) RCT V 133678-80-5  
PRO C 124909-09-7, X 133678-83-8, Y 141045-40-1  
CAT 121-44-8 Et3N, 20667-12-3 Ag2O  
SOL 67-56-1 MeOH  
NTE key step

RX(22) RCT X 133678-83-8

STAGE(1)  
RGT Q 16940-66-2 NaBH4  
SOL 64-17-5 EtOH

STAGE(2)  
RGT R 7647-01-0 HCl  
SOL 7732-18-5 Water  
PRO BI 141045-53-6, BJ 141116-75-8

RX(30) RCT BI 141045-53-6

STAGE(1)  
SOL 108-88-3 PhMe

STAGE(2)  
RGT BX 603-35-0 PPh3, BY 288-32-4 1H-Imidazole, BZ 7553-56-2 I2

STAGE(3)  
RGT CA 144-55-8 NaHCO3  
SOL 7732-18-5 Water

STAGE(4)  
RGT BZ 7553-56-2 I2

STAGE(5)  
RGT CB 7772-98-7 Na2S2O3  
SOL 7732-18-5 Water  
PRO BK 141045-55-8

RX(23) RCT BK 141045-55-8  
RGT BM 6674-22-2 DBU  
PRO BL 141045-59-2  
SOL 109-99-9 THF

RX(24) RCT BL 141045-59-2, BN 917-54-4

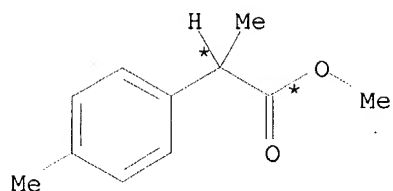
STAGE(1)  
SOL 60-29-7 Et2O

STAGE(2)  
RGT AK 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
PRO BG 141045-52-5, BO 141045-60-5, BP 141045-61-6

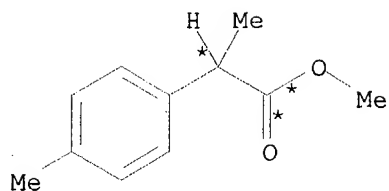
RX(441) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(9), RX(22), RX(30),  
RX(23), RX(24)

RX(441) 4 E + 4 F + 4 U + 5 BN ==> BG + BO +

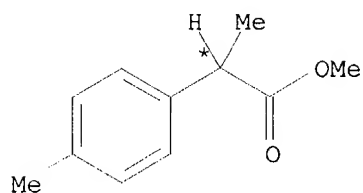
BP



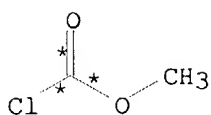
E



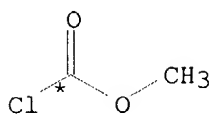
2 E



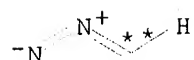
E



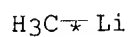
3 F



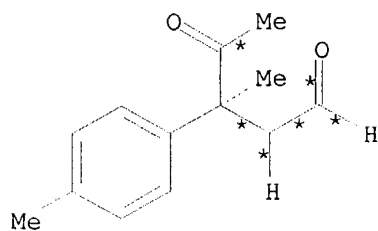
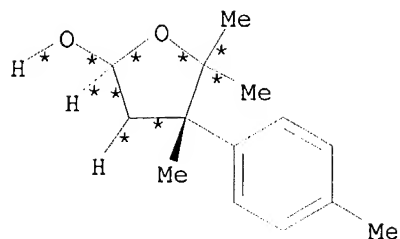
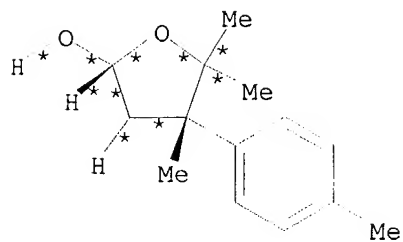
F



4 U



5 BN

9  
STEPS  
→BG  
YIELD 50%BO  
YIELD 20% (67)BP  
YIELD 20% (33)

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi  
SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1  
PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>O

RX(9) RCT V 133678-80-5  
RGT R 7647-01-0 HCl  
PRO X 133678-83-8, Y 141045-40-1  
SOL 7732-18-5 Water, 109-99-9 THF

RX(22) RCT X 133678-83-8

STAGE(1)

RGT Q 16940-66-2 NaBH<sub>4</sub>  
SOL 64-17-5 EtOH

STAGE(2)

RGT R 7647-01-0 HCl  
SOL 7732-18-5 Water  
PRO BI 141045-53-6, BJ 141116-75-8

RX(30) RCT BI 141045-53-6

STAGE(1)

SOL 108-88-3 PhMe

STAGE(2)

RGT BX 603-35-0 PPh<sub>3</sub>, BY 288-32-4 1H-Imidazole, BZ 7553-56-2 I<sub>2</sub>

STAGE(3)

RGT CA 144-55-8 NaHCO<sub>3</sub>  
SOL 7732-18-5 Water

STAGE(4)

RGT BZ 7553-56-2 I<sub>2</sub>

STAGE(5)

RGT CB 7772-98-7 Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>  
SOL 7732-18-5 Water  
PRO BK 141045-55-8

RX(23) RCT BK 141045-55-8  
 RGT BM 6674-22-2 DBU  
 PRO BL 141045-59-2  
 SOL 109-99-9 THF

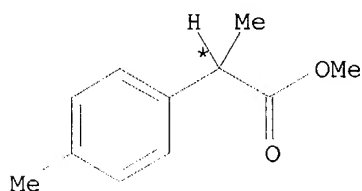
RX(24) RCT BL 141045-59-2, BN 917-54-4

STAGE(1)  
 SOL 60-29-7 Et2O

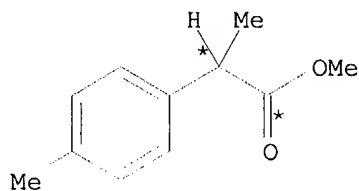
STAGE(2)  
 RGT AK 12125-02-9 NH4Cl  
 SOL 7732-18-5 Water  
 PRO BG 141045-52-5, BO 141045-60-5, BP 141045-61-6

RX(469) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(7), RX(32), RX(22),  
 RX(30), RX(23), RX(24)

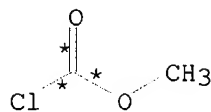
RX(469) 5 E + 5 F + 5 U + 5 BN ==> BG + BO +  
 BP



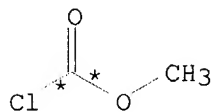
3 E



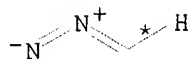
2 E



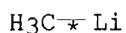
3 F



2 F

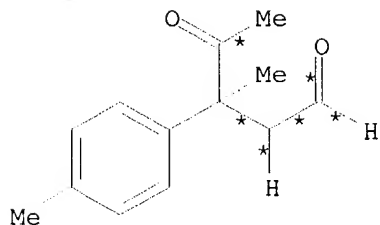


5 U

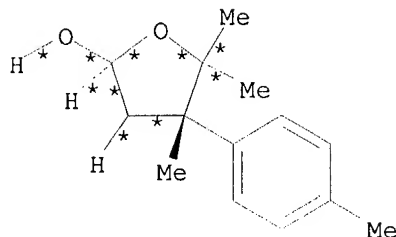


5 BN

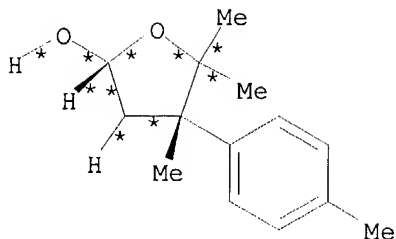
10  
 STEPS  
 →



BG  
 YIELD 50%



BO  
 YIELD 20% (67)



BP

YIELD 20% (33)

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi

SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1

PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>O

RX(7) RCT V 133678-80-5  
PRO C 124909-09-7, X 133678-83-8, Y 141045-40-1  
CAT 121-44-8 Et<sub>3</sub>N, 20667-12-3 Ag<sub>2</sub>O  
SOL 67-56-1 MeOH  
NTE key step

RX(32) RCT Y 141045-40-1  
PRO X 133678-83-8  
SOL 865-49-6 CDCl<sub>3</sub>

RX(22) RCT X 133678-83-8

STAGE(1)

RGT Q 16940-66-2 NaBH<sub>4</sub>

SOL 64-17-5 EtOH

STAGE(2)

RGT R 7647-01-0 HCl

SOL 7732-18-5 Water

PRO BI 141045-53-6, BJ 141116-75-8



RX(30) RCT BI 141045-53-6

STAGE(1)

SOL 108-88-3 PhMe

STAGE(2)

RGT BX 603-35-0 PPh3, BY 288-32-4 1H-Imidazole, BZ 7553-56-2 I2

STAGE(3)

RGT CA 144-55-8 NaHCO3

SOL 7732-18-5 Water

STAGE(4)

RGT BZ 7553-56-2 I2

STAGE(5)

RGT CB 7772-98-7 Na2S2O3

SOL 7732-18-5 Water

PRO BK 141045-55-8

RX(23) RCT BK 141045-55-8

RGT BM 6674-22-2 DBU

PRO BL 141045-59-2

SOL 109-99-9 THF

RX(24) RCT BL 141045-59-2, BN 917-54-4

STAGE(1)

SOL 60-29-7 Et2O

STAGE(2)

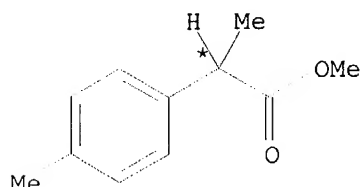
RGT AK 12125-02-9 NH4Cl

SOL 7732-18-5 Water

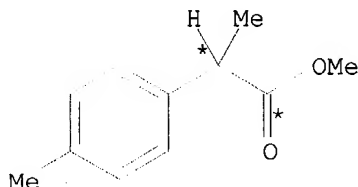
PRO BG 141045-52-5, BO 141045-60-5, BP 141045-61-6

RX(471) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(9), RX(32), RX(22),  
RX(30), RX(23), RX(24)

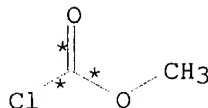
RX(471) 5 E + 5 F + 5 U + 5 BN ==> BG + BO +  
BP



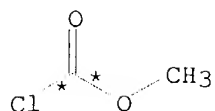
3 E



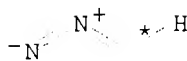
2 E



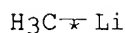
3 F



2 F

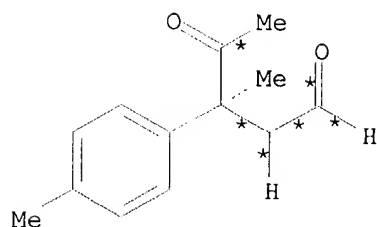


5 U

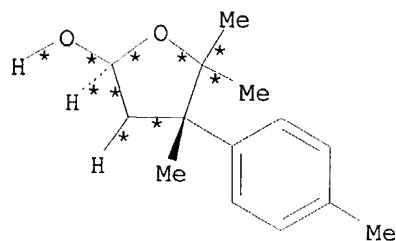


5 BN

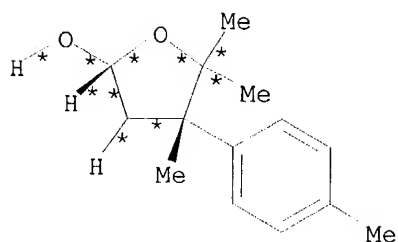
10  
STEPS  
→



BG  
YIELD 50%



BO  
YIELD 20% (67)



BP  
YIELD 20% (33)

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi  
SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1  
PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>O

RX(9) RCT V 133678-80-5  
RGT R 7647-01-0 HCl  
PRO X 133678-83-8, Y 141045-40-1  
SOL 7732-18-5 Water, 109-99-9 THF

RX(32) RCT Y 141045-40-1

PRO X 133678-83-8  
SOL 865-49-6 CDC13

RX(22) RCT X 133678-83-8

STAGE(1)  
RGT Q 16940-66-2 NaBH4  
SOL 64-17-5 EtOH

STAGE(2)  
RGT R 7647-01-0 HCl  
SOL 7732-18-5 Water  
PRO BI 141045-53-6, BJ 141116-75-8

RX(30) RCT BI 141045-53-6

STAGE(1)  
SOL 108-88-3 PhMe

STAGE(2)  
RGT BX 603-35-0 PPh3, BY 288-32-4 1H-Imidazole, BZ 7553-56-2 I2

STAGE(3)  
RGT CA 144-55-8 NaHCO3  
SOL 7732-18-5 Water

STAGE(4)  
RGT BZ 7553-56-2 I2

STAGE(5)  
RGT CB 7772-98-7 Na2S2O3  
SOL 7732-18-5 Water  
PRO BK 141045-55-8

RX(23) RCT BK 141045-55-8  
RGT BM 6674-22-2 DBU  
PRO BL 141045-59-2  
SOL 109-99-9 THF

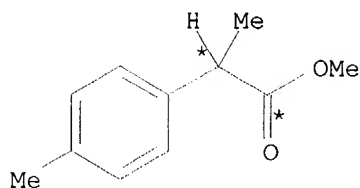
RX(24) RCT BL 141045-59-2, BN 917-54-4

STAGE(1)  
SOL 60-29-7 Et2O

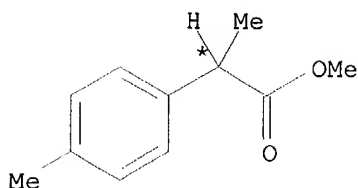
STAGE(2)  
RGT AK 12125-02-9 NH4Cl  
SOL 7732-18-5 Water  
PRO BG 141045-52-5, BO 141045-60-5, BP 141045-61-6

RX(472) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(7), RX(16), RX(17),  
RX(18), RX(19), RX(20)

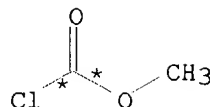
RX(472) 4 E + 4 F + 4 U + 3 AU + 2 AH ==> BG



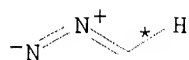
E



3 E



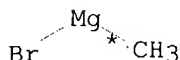
4 F



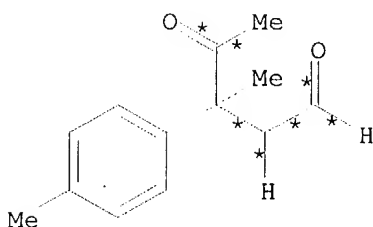
4 U



3 AU



2 AH

10  
STEPS  
→BG  
YIELD 97%

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi  
SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1  
PRO G 127047-04-5RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 BenzeneRX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>ORX(7) RCT V 133678-80-5  
PRO C 124909-09-7, X 133678-83-8, Y 141045-40-1

CAT 121-44-8 Et3N, 20667-12-3 Ag2O  
 SOL 67-56-1 MeOH  
 NTE key step

RX(16) RCT X 133678-83-8, AU 540-63-6  
 PRO AV 141045-46-7  
 CAT 109-63-7 BF3-Et2O  
 SOL 75-09-2 CH2Cl2

RX(17) RCT AV 141045-46-7  
 RGT AZ 7440-02-0 Ni  
 PRO AX 141116-74-7, AY 141045-47-8  
 SOL 64-17-5 EtOH  
 NTE Raney Ni

RX(18) RCT AX 141116-74-7  
 RGT BC 1191-15-7 AlH(Bu-i)2  
 PRO BA 141045-48-9, BB 141045-49-0  
 SOL 108-88-3 PhMe

RX(19) RCT BA 141045-48-9, AH 75-16-1  
 PRO BE 141045-50-3, BF 141045-51-4  
 SOL 60-29-7 Et2O

RX(20) RCT BE 141045-50-3

# STAGE(1)

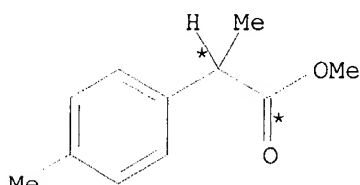
RGT AM 79-37-8 (COCl)2, AN 67-68-5 DMSO  
 SOL 75-09-2 CH2Cl2

# STAGE(2)

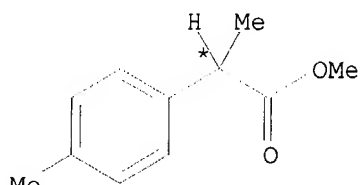
RGT P 121-44-8 Et3N  
 PRO BG 141045-52-5  
 NTE STEREOISOMERIC REACTANT PRESENT

RX(473) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(7), RX(16), RX(17),  
 RX(18), RX(19), RX(35)

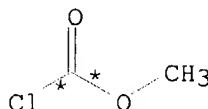
RX(473) 4 E + 4 F + 4 U + 3 AU + 2 AH ==> BG



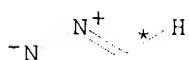
2 E



2 E



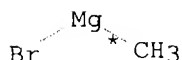
4 F



4 U

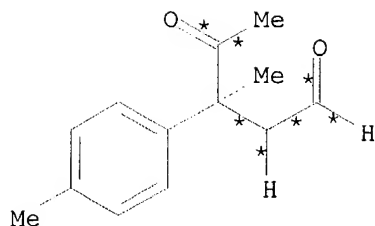


3 AU



2 AH

10  
 STEPS  
 >



BG  
YIELD 97%

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi  
SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1  
PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>O

RX(7) RCT V 133678-80-5  
PRO C 124909-09-7, X 133678-83-8, Y 141045-40-1  
CAT 121-44-8 Et<sub>3</sub>N, 20667-12-3 Ag<sub>2</sub>O  
SOL 67-56-1 MeOH  
NTE key step

RX(16) RCT X 133678-83-8, AU 540-63-6  
PRO AV 141045-46-7  
CAT 109-63-7 BF<sub>3</sub>-Et<sub>2</sub>O  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(17) RCT AV 141045-46-7  
RGT AZ 7440-02-0 Ni  
PRO AX 141116-74-7, AY 141045-47-8  
SOL 64-17-5 EtOH  
NTE Raney Ni

RX(18) RCT AX 141116-74-7  
RGT BC 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO BA 141045-48-9, BB 141045-49-0  
SOL 108-88-3 PhMe

RX(19) RCT BA 141045-48-9, AH 75-16-1  
 PRO BE 141045-50-3, BF 141045-51-4  
 SOL 60-29-7 Et2O

RX(35) RCT BF 141045-51-4

STAGE(1)

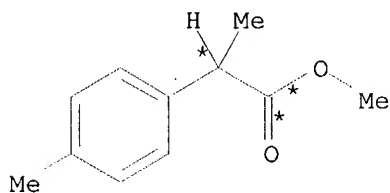
RGT AM 79-37-8 (COCl)<sub>2</sub>, AN 67-68-5 DMSO  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

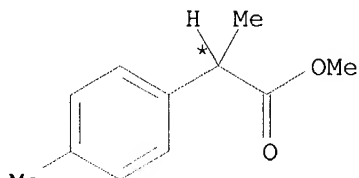
RGT P 121-44-8 Et<sub>3</sub>N  
 PRO BG 141045-52-5  
 NTE STEREOISOMERIC REACTANT PRESENT

RX(474) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(9), RX(16), RX(17),  
 RX(18), RX(19), RX(20)

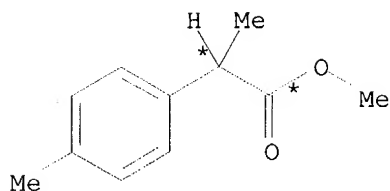
RX(474) 3 E + 3 F + 3 U + 3 AU + 2 AH ==> BG



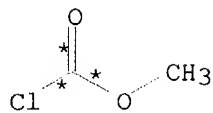
E



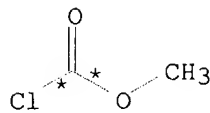
E



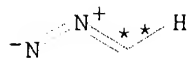
E



2 F



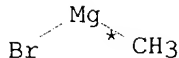
F



3 U

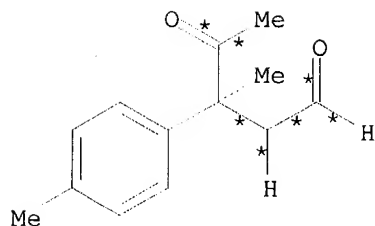


3 AU



2 AH

10  
 STEPS  
 →



BG  
YIELD 97%

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi  
SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1  
PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>O

RX(9) RCT V 133678-80-5  
RGT R 7647-01-0 HCl  
PRO X 133678-83-8, Y 141045-40-1  
SOL 7732-18-5 Water, 109-99-9 THF

RX(16) RCT X 133678-83-8, AU 540-63-6  
PRO AV 141045-46-7  
CAT 109-63-7 BF<sub>3</sub>-Et<sub>2</sub>O  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(17) RCT AV 141045-46-7  
RGT AZ 7440-02-0 Ni  
PRO AX 141116-74-7, AY 141045-47-8  
SOL 64-17-5 EtOH  
NTE Raney Ni

RX(18) RCT AX 141116-74-7  
RGT BC 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO BA 141045-48-9, BB 141045-49-0  
SOL 108-88-3 PhMe

RX(19) RCT BA 141045-48-9, AH 75-16-1



PRO BE 141045-50-3, BF 141045-51-4  
SOL 60-29-7 Et2O

RX(20) RCT BE 141045-50-3

STAGE(1)

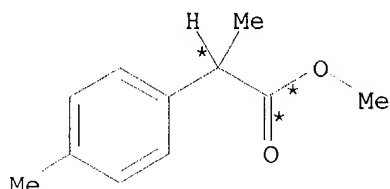
RGT AM 79-37-8 (COCl)<sub>2</sub>, AN 67-68-5 DMSO  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

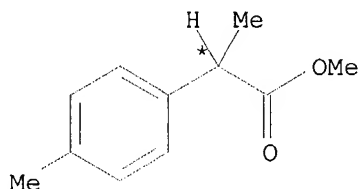
RGT P 121-44-8 Et<sub>3</sub>N  
PRO BG 141045-52-5  
NTE STEREOISOMERIC REACTANT PRESENT

RX(475) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(9), RX(16), RX(17),  
RX(18), RX(19), RX(35)

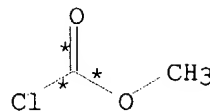
RX(475) 3 E + 3 F + 3 U + 3 AU + 2 AH ==> BG



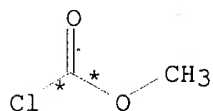
2 E



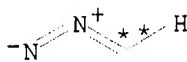
E



2 F



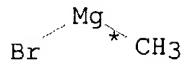
F



3 U

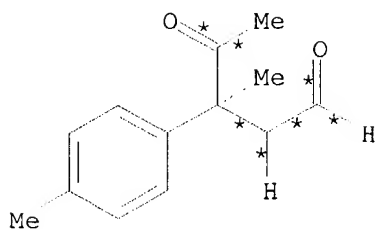


3 AU



2 AH

10  
STEPS



BG  
YIELD 97%

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi  
SOL 109-99-9 THF

## STAGE(2)

RCT F 79-22-1  
PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>O

RX(9) RCT V 133678-80-5  
RGT R 7647-01-0 HCl  
PRO X 133678-83-8, Y 141045-40-1  
SOL 7732-18-5 Water, 109-99-9 THF

RX(16) RCT X 133678-83-8, AU 540-63-6  
PRO AV 141045-46-7  
CAT 109-63-7 BF<sub>3</sub>-Et<sub>2</sub>O  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(17) RCT AV 141045-46-7  
RGT AZ 7440-02-0 Ni  
PRO AX 141116-74-7, AY 141045-47-8  
SOL 64-17-5 EtOH  
NTE Raney Ni

RX(18) RCT AX 141116-74-7  
RGT BC 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO BA 141045-48-9, BB 141045-49-0  
SOL 108-88-3 PhMe

RX(19) RCT BA 141045-48-9, AH 75-16-1  
PRO BE 141045-50-3, BF 141045-51-4  
SOL 60-29-7 Et<sub>2</sub>O

RX(35) RCT BF 141045-51-4

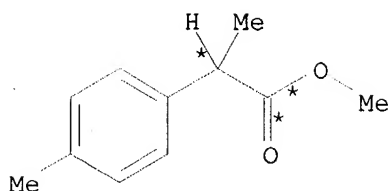
## STAGE(1)

RGT AM 79-37-8 (COCl)<sub>2</sub>, AN 67-68-5 DMSO  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

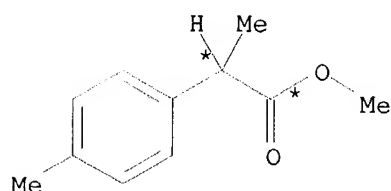
## STAGE(2)

RGT P 121-44-8 Et<sub>3</sub>N  
PRO BG 141045-52-5  
NTE STEREOISOMERIC REACTANT PRESENT

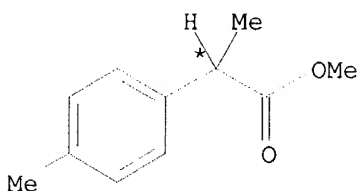
RX(532) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(7), RX(32), RX(16),  
RX(17), RX(18), RX(19), RX(20)  
RX(532) 5 E + 5 F + 5 U + 3 AU + 2 AH ==> BG



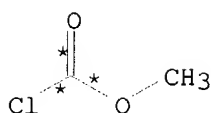
E



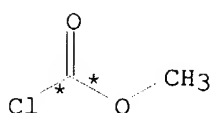
E



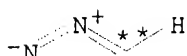
3 E



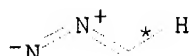
2 F



3 F



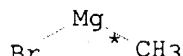
U



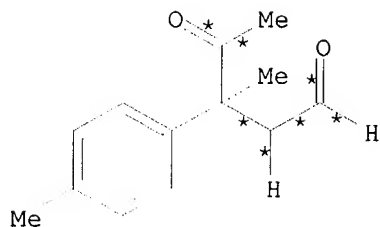
4 U



3 AU



2 AH

11  
STEPS  
→BG  
YIELD 97%

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr2NH, I 109-72-8 BuLi  
SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1  
PRO G 127047-04-5RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water

NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>O

RX(7) RCT V 133678-80-5  
PRO C 124909-09-7, X 133678-83-8, Y 141045-40-1  
CAT 121-44-8 Et<sub>3</sub>N, 20667-12-3 Ag<sub>2</sub>O  
SOL 67-56-1 MeOH  
NTE key step

RX(32) RCT Y 141045-40-1  
PRO X 133678-83-8  
SOL 865-49-6 CDCl<sub>3</sub>

RX(16) RCT X 133678-83-8, AU 540-63-6  
PRO AV 141045-46-7  
CAT 109-63-7 BF<sub>3</sub>-Et<sub>2</sub>O  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(17) RCT AV 141045-46-7  
RGT AZ 7440-02-0 Ni  
PRO AX 141116-74-7, AY 141045-47-8  
SOL 64-17-5 EtOH  
NTE Raney Ni

RX(18) RCT AX 141116-74-7  
RGT BC 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO BA 141045-48-9, BB 141045-49-0  
SOL 108-88-3 PhMe

RX(19) RCT BA 141045-48-9, AH 75-16-1  
PRO BE 141045-50-3, BF 141045-51-4  
SOL 60-29-7 Et<sub>2</sub>O

RX(20) RCT BE 141045-50-3

## STAGE(1)

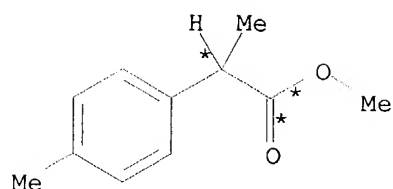
RGT AM 79-37-8 (COCl)<sub>2</sub>, AN 67-68-5 DMSO  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

## STAGE(2)

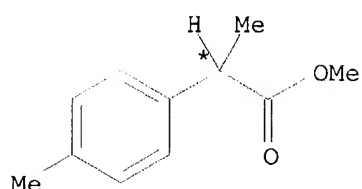
RGT P 121-44-8 Et<sub>3</sub>N  
PRO BG **141045-52-5**  
NTE STEREOISOMERIC REACTANT PRESENT

RX(533) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(7), RX(32), RX(16),  
RX(17), RX(18), RX(19), RX(35)

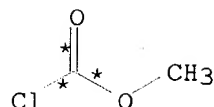
RX(533) 5 E + 5 F + 5 U + 3 AU + 2 AH ==> BG



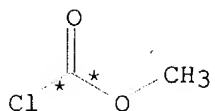
2 E



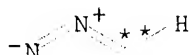
3 E



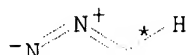
2 F



3 F



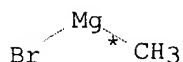
U



4 U

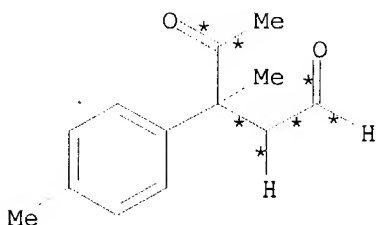


3 AU



2 AH

11  
STEPS  
→



BG  
YIELD 97%

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi

SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1

PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7

SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et2O

RX(7) RCT V 133678-80-5  
PRO C 124909-09-7, X 133678-83-8, Y 141045-40-1  
CAT 121-44-8 Et3N, 20667-12-3 Ag2O  
SOL 67-56-1 MeOH  
NTE key step

RX(32) RCT Y 141045-40-1  
PRO X 133678-83-8  
SOL 865-49-6 CDCl3

RX(16) RCT X 133678-83-8, AU 540-63-6  
PRO AV 141045-46-7  
CAT 109-63-7 BF3-Et2O  
SOL 75-09-2 CH2Cl2

RX(17) RCT AV 141045-46-7  
RGT AZ 7440-02-0 Ni  
PRO AX 141116-74-7, AY 141045-47-8  
SOL 64-17-5 EtOH  
NTE Raney Ni

RX(18) RCT AX 141116-74-7  
RGT BC 1191-15-7 AlH(Bu-i)2  
PRO BA 141045-48-9, BB 141045-49-0  
SOL 108-88-3 PhMe

RX(19) RCT BA 141045-48-9, AH 75-16-1  
PRO BE 141045-50-3, BF 141045-51-4  
SOL 60-29-7 Et2O

RX(35) RCT BF 141045-51-4

STAGE(1)

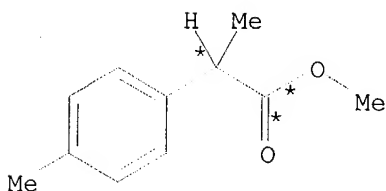
RGT AM 79-37-8 (COCl)2, AN 67-68-5 DMSO  
SOL 75-09-2 CH2Cl2

STAGE(2)

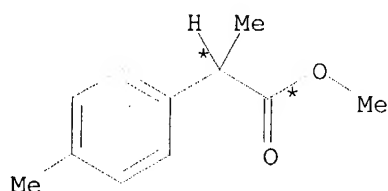
RGT P 121-44-8 Et3N  
PRO BG 141045-52-5  
NTE STEREOISOMERIC REACTANT PRESENT

RX(534) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(9), RX(32), RX(16),  
RX(17), RX(18), RX(19), RX(20)

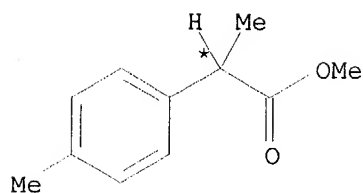
RX(534) 4 E + 4 F + 4 U + 3 AU + 2 AH ==> BG



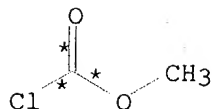
E



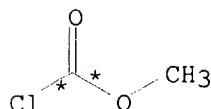
E



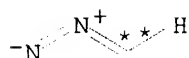
2 E



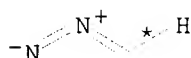
2 F



2 F



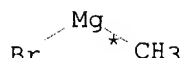
U



3 U

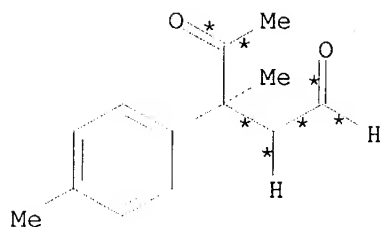


3 AU



2 AH

11  
STEPS  
➔



BG  
YIELD 97%

RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi

SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1

PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>O

RX(9) RCT V 133678-80-5

RGT R 7647-01-0 HCl  
 PRO X 133678-83-8, Y 141045-40-1  
 SOL 7732-18-5 Water, 109-99-9 THF

RX(32) RCT Y 141045-40-1  
 PRO X 133678-83-8  
 SOL 865-49-6 CDCl3

RX(16) RCT X 133678-83-8, AU 540-63-6  
 PRO AV 141045-46-7  
 CAT 109-63-7 BF3-Et2O  
 SOL 75-09-2 CH2Cl2

RX(17) RCT AV 141045-46-7  
 RGT AZ 7440-02-0 Ni  
 PRO AX 141116-74-7, AY 141045-47-8  
 SOL 64-17-5 EtOH  
 NTE Raney Ni

RX(18) RCT AX 141116-74-7  
 RGT BC 1191-15-7 AlH(Bu-i)2  
 PRO BA 141045-48-9, BB 141045-49-0  
 SOL 108-88-3 PhMe

RX(19) RCT BA 141045-48-9, AH 75-16-1  
 PRO BE 141045-50-3, BF 141045-51-4  
 SOL 60-29-7 Et2O

RX(20) RCT BE 141045-50-3

STAGE(1)

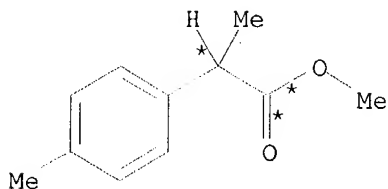
RGT AM 79-37-8 (COCl)2, AN 67-68-5 DMSO  
 SOL 75-09-2 CH2Cl2

STAGE(2)

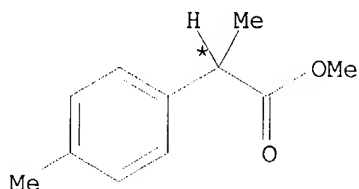
RGT P 121-44-8 Et3N  
 PRO BG 141045-52-5  
 NTE STEREOISOMERIC REACTANT PRESENT

RX(535) OF 573 COMPOSED OF RX(3), RX(4), RX(31), RX(6), RX(9), RX(32), RX(16),  
 RX(17), RX(18), RX(19), RX(35)

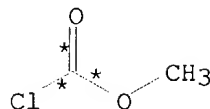
RX(535) 4 E + 4 F + 4 U + 3 AU + 2 AH ==> BG



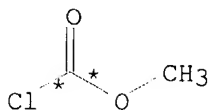
2 E



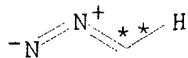
2 E



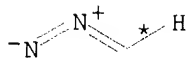
2 F



2 F



U

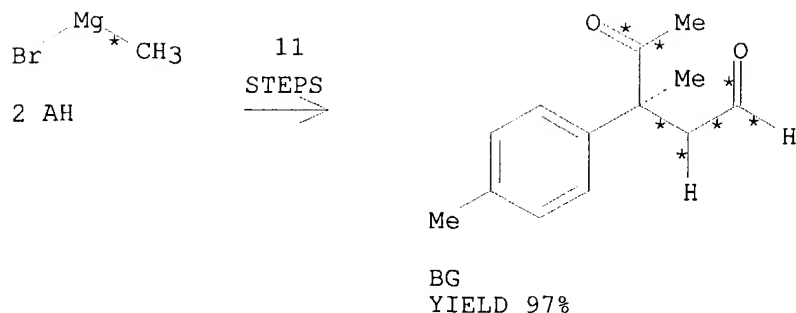


3 U



3 AU





RX(3) RCT E 79443-97-3

STAGE(1)

RGT H 108-18-9 i-Pr<sub>2</sub>NH, I 109-72-8 BuLi  
SOL 109-99-9 THF

STAGE(2)

RCT F 79-22-1  
PRO G 127047-04-5

RX(4) RCT G 127047-04-5  
RGT L 1310-73-2 NaOH  
PRO K 127047-05-6  
CAT 9013-79-0 Esterase  
SOL 7732-18-5 Water  
NTE regioselective enzymic key step; (pH 7.2)

RX(31) RCT K 127047-05-6  
RGT AM 79-37-8 (COCl)<sub>2</sub>  
PRO T 141045-62-7  
SOL 71-43-2 Benzene

RX(6) RCT T 141045-62-7, U 334-88-3  
PRO V 133678-80-5  
SOL 60-29-7 Et<sub>2</sub>O

RX(9) RCT V 133678-80-5  
RGT R 7647-01-0 HCl  
PRO X 133678-83-8, Y 141045-40-1  
SOL 7732-18-5 Water, 109-99-9 THF

RX(32) RCT Y 141045-40-1  
PRO X 133678-83-8  
SOL 865-49-6 CDCl<sub>3</sub>

RX(16) RCT X 133678-83-8, AU 540-63-6  
PRO AV 141045-46-7  
CAT 109-63-7 BF<sub>3</sub>-Et<sub>2</sub>O  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

RX(17) RCT AV 141045-46-7  
RGT AZ 7440-02-0 Ni  
PRO AX 141116-74-7, AY 141045-47-8  
SOL 64-17-5 EtOH  
NTE Raney Ni

RX(18) RCT AX 141116-74-7  
RGT BC 1191-15-7 AlH(Bu-i)<sub>2</sub>  
PRO BA 141045-48-9, BB 141045-49-0  
SOL 108-88-3 PhMe

RX(19) RCT BA 141045-48-9, AH 75-16-1  
PRO BE 141045-50-3, BF 141045-51-4  
SOL 60-29-7 Et<sub>2</sub>O

RX(35) RCT BF 141045-51-4

STAGE(1)

RGT AM 79-37-8 (COCl)<sub>2</sub>, AN 67-68-5 DMSO  
SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

STAGE(2)

RGT P 121-44-8 Et<sub>3</sub>N  
PRO BG **141045-52-5**  
NTE STEREOISOMERIC REACTANT PRESENT

L20 ANSWER 5 OF 6 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 110:114498 CASREACT

TITLE: Electrophile-initiated conversion of a prostaglandin endoperoxide model compound to the thromboxane B skeleton

AUTHOR(S): Takahashi, Kimio; Kishi, Morio

CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan

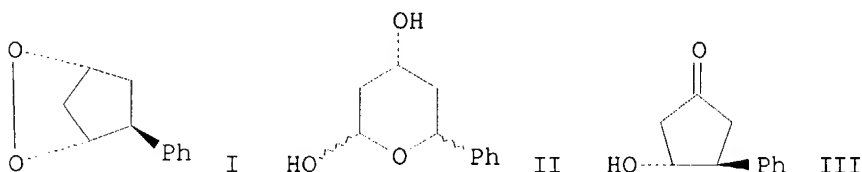
SOURCE: Tetrahedron Letters (1988), 29(36), 4595-6

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

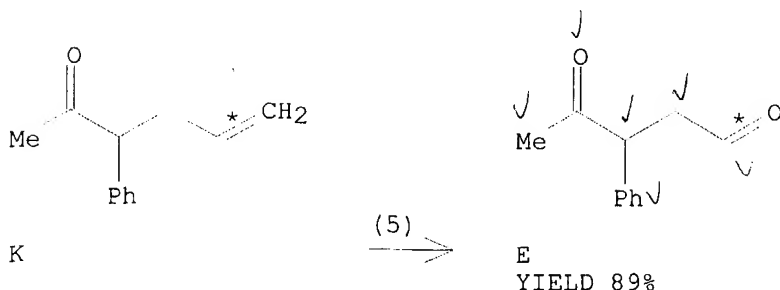
LANGUAGE: English

GI



AB Reaction of the simplified prostaglandin endoperoxide model I with ferric or cupric ion afforded the lactols II contg. the thromboxane B ring moiety, along with ketol III, MeCOCH<sub>2</sub>CHPhCHO, and MeCOCHPhCH<sub>2</sub>CHO.

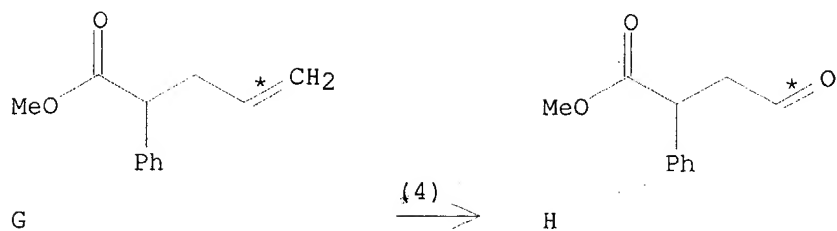
RX(5) OF 7 ...K ==> E



PRO E 89969-01-7

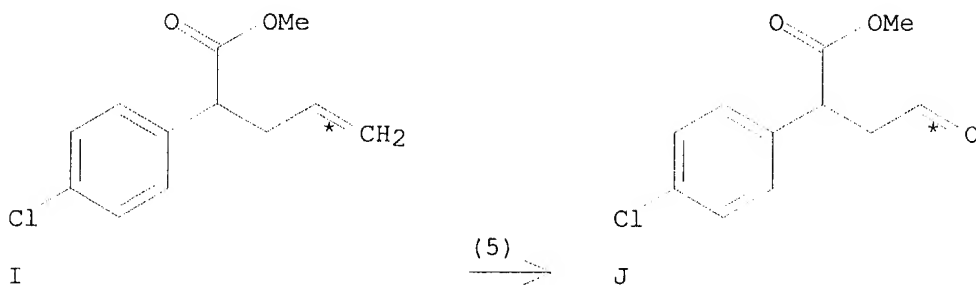
R1C(Br)C=C(c1ccc(R)cc1)C(=O)O

Searched by Barb O'Bryen, STIC 571-272-2518



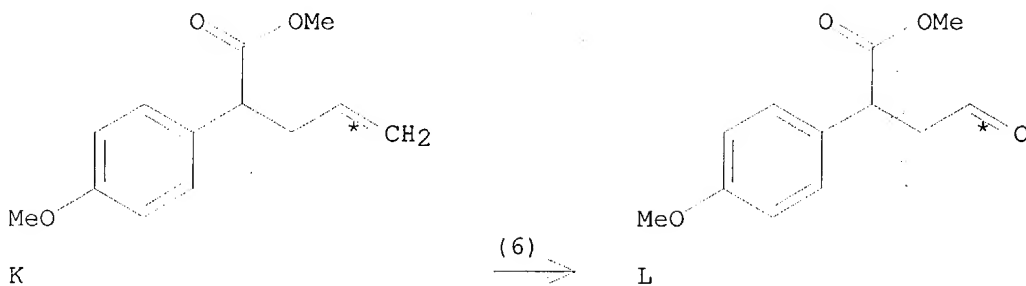
RX(4)      RCT   G 14815-73-7  
             PRO   H 67031-12-3  
             SOL   75-18-3 Me2S

RX(5) OF 26      I ==> J...



RX(5)      RCT   I 67031-09-8  
             PRO   J 67031-16-7  
             SOL   75-18-3 Me2S

RX(6) OF 26      K ==> L



RX(6)      RCT   K 67031-10-1  
             PRO   L 67031-18-9  
             SOL   75-18-3 Me2S

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